Multiscale study of hydrogen isotopes structural properties in solid phase in the context of inertial fusion target manufacturing.

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INDUSTRIALES
ETSII | UPM

Presentation

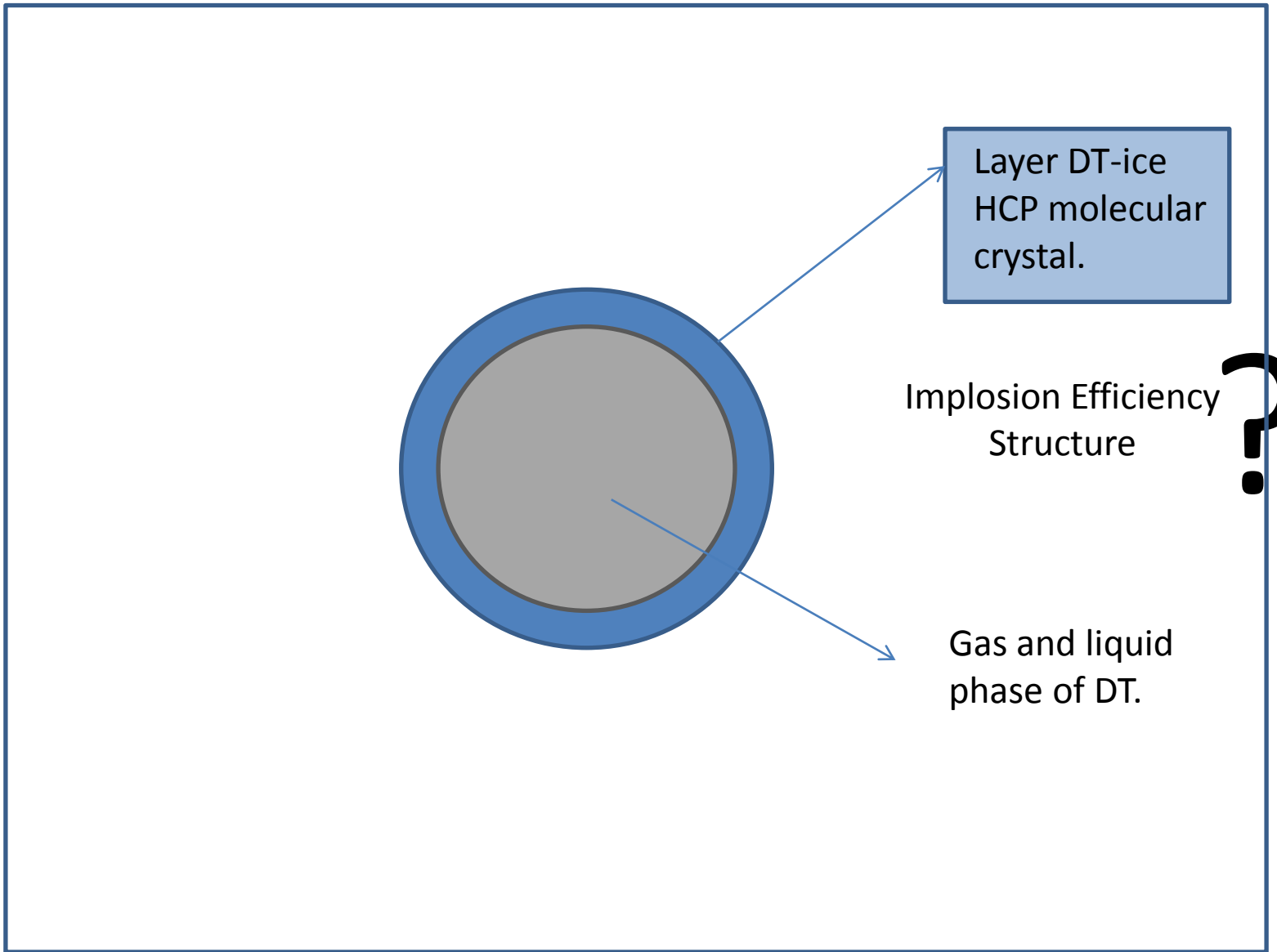
- Problems
- Methodology
- Results
- Conclusions

Target ICF

acknowledgment:http://www.hiper-laser.org/

Target ICF

acknowledgment:http://www.hiper-laser.org/



Requirements ICF

Designing the ignition and high-gain targets for inertial confinement fusion (ICF) requires a **condensed uniform layer of the hydrogen fuel** on the inner surface of a spherical polymer shell. The fuel layers have to be highly uniform in **thickness and roughness**. (Aleksandrova 2008)

To **direct-drive** the parameters of the cryogenic fuel layer should satisfy the following quality criteria (Aleksandrova 2007):

1) **thickness variation**, no more than 2 %.

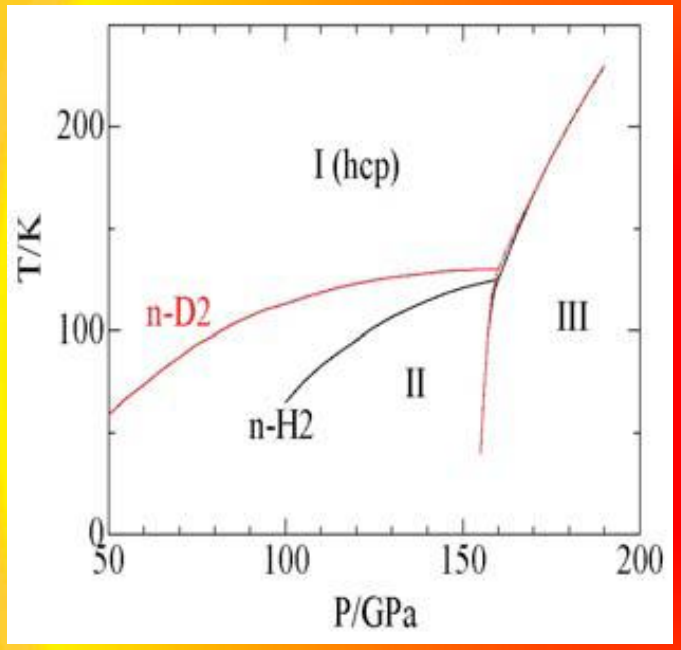
2) **Free surface roughness**, no more than 0,1 um,

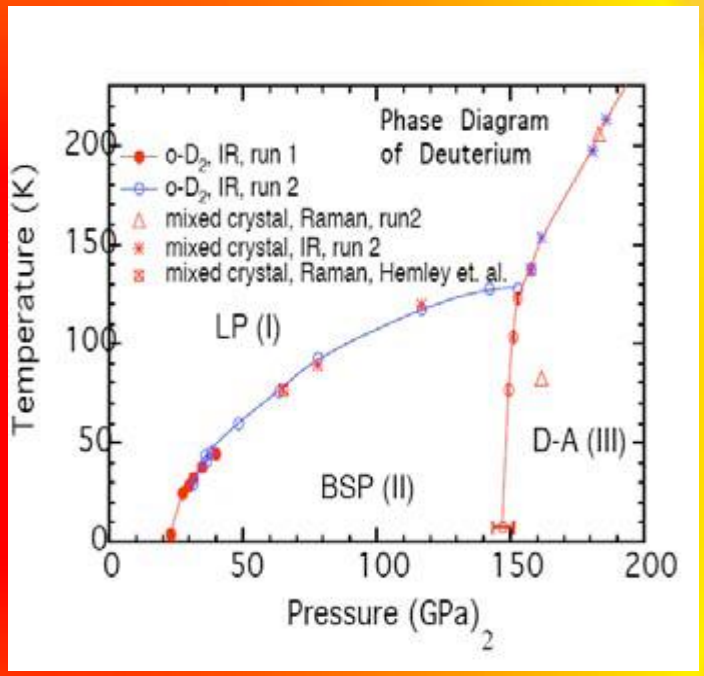
3) **Temperature** ~1.5-1.8 K lower than the fuel triple point.

In OMEGA is necesary 100 to 1000 atm **pressure in target pellet**. Since the shell itself does not withstand than 5-40 atm at T=300 K, it is evident that this high internal pressure would inevitably result in its rupture. (Aleksandrova 2007)

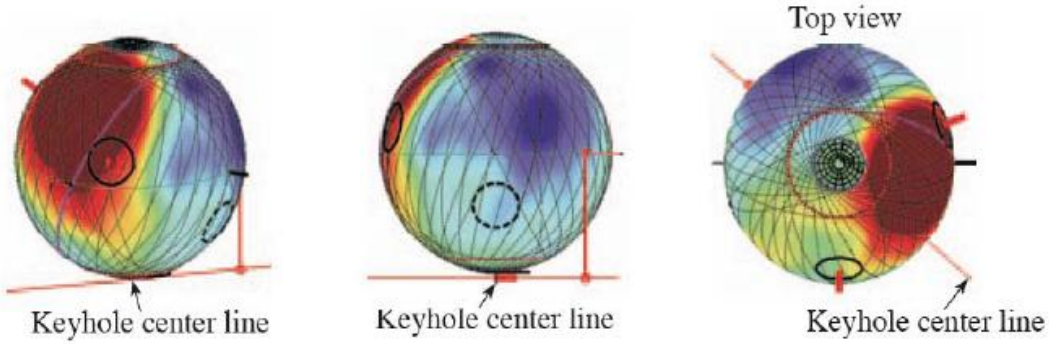
Low Degradation: During its delivery from the formation module and positioning in the irradiation zone, the target is subject to thermal and mechanical stresses. The cryogenic fuel layer is the most susceptible component of the target. (Aleksandrova 2007)

Phase Diagram

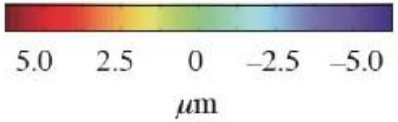


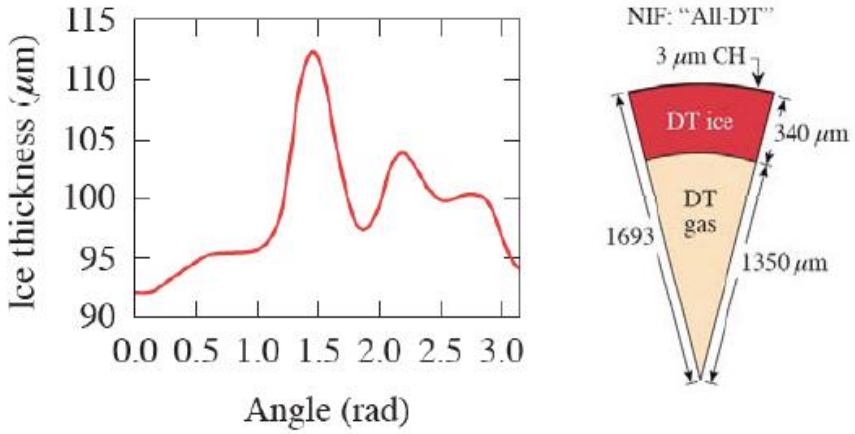


- Phase diagram for the deuterium and hydrogen, on the left shows the difference between H_2 and D_2 (Kawamura 2008) .In the right shows different results for the D_2 (Silvera 2010)



Aleksandrova 2004





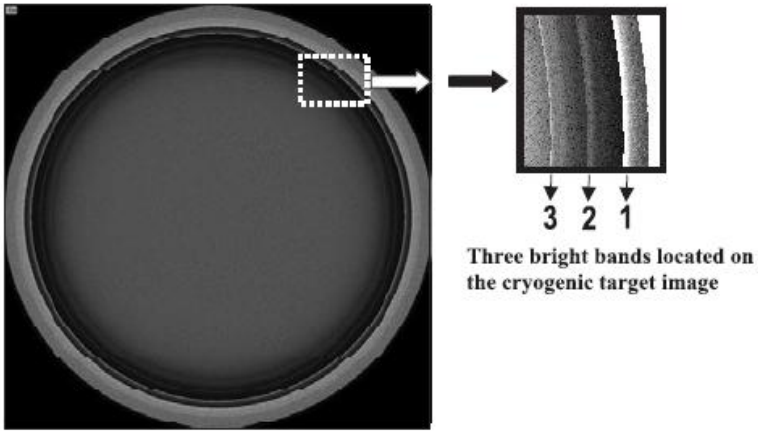


Figure 6. The BBP algorithm for three-dimensional reconstruction of the inner target surface based on the analysis of the bright band structure and localization in the target images obtained from backlit shadowgraphy.

Harding 2004

The image above shows the difference in thickness for a sphere of DT ice, red is the thickest layer and a thin purple. Below is a sample calculation of the ratio thickness vs. angle, and a diagram of the layered structure of the sphere of DT ice (Harding 2004).

Problems in Target pellet for ICF

Phase Transicions (Koziozemski 2010). Local perturbations are a much more serious problem for the damage of the cryogenic layer than its distortion along the thickness (Aleksandrova 2007).

Crystal structure to high pressure (Mc Mahon 2011), **Sound propagations** in molecular crystal??? In hexagonal crystal the sound speed depends on sound wave line about the crystallographic axes. In molecular crystal the mechanism of heat conduction is mainly connected with lattice conductivity, which depends on sound speed. (Korosheva 2008)

Stress to structure (Aleksandrova 2008), *Is nessesary stress calculation for the target in delivery condictions*. This study can be classified into the three structural states: a) near-nano (0.1-0.3 um) fine-grained crystalline. b) Nanocrystalline state (grain size <= 100 nm). c) amorphous state (~1 nm).

Size effect: When the material sizes approach the nanometer range, the materials exhibit peculiar and interesting mechanical and physical properties, e.g., increased mechanical strength, enhanced diffusivity, and higher specific heat and electrical resistivity compared to the conventional coarse-grained counterparts. (Aleksandrova 2008)

Dopant and uniformed layer (Aleksandrova 2007). Introduction of certain dopants makes it possible to obtain a solid cryogenic layer inside the microsphere, which layer remains transparent for several heating-cooling cycles within the temperature range from 5 K to the triple point of the isotope.

Objects

- Study the phase transtion in hydrogen isotopes.
- Obtain the crystal structure in these phases
- Obtain the stress tensor, and strain tensor to define the elastic constant of hydrogen isotopes
- Study size effect in nanostructures of hydrogen
- Study the hydrogen crystal structure with dopands.

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Multiscale Methodology

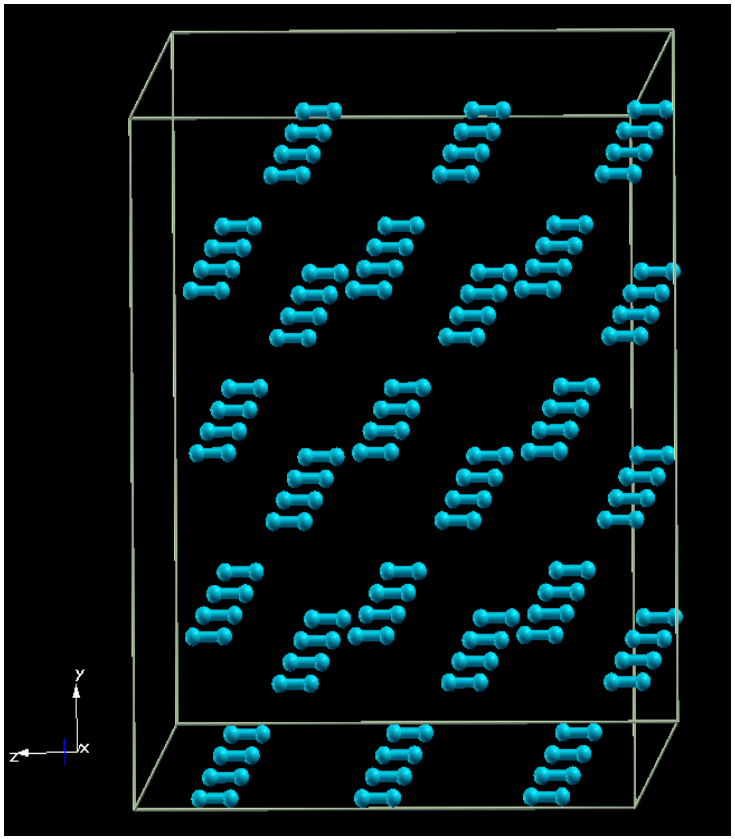
The methodology is divided in three areas for the multiscale study:

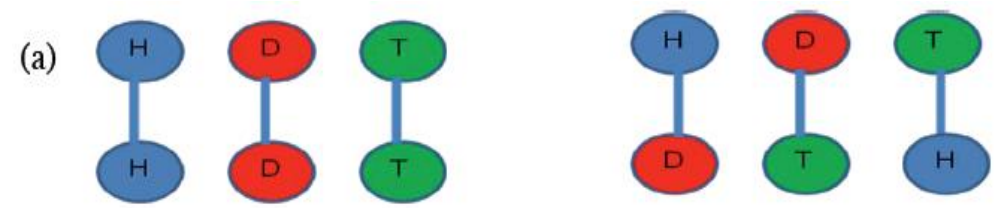
1) Ab initio calculations of the nanostructure
2) Molecular Quantum Dynamics of the Nanostructures
3) Simulation in continuous media

Ab initio program is **SIESTA** (**Spanish Initiative for Electronic Simulations with Thousands of Atoms**)

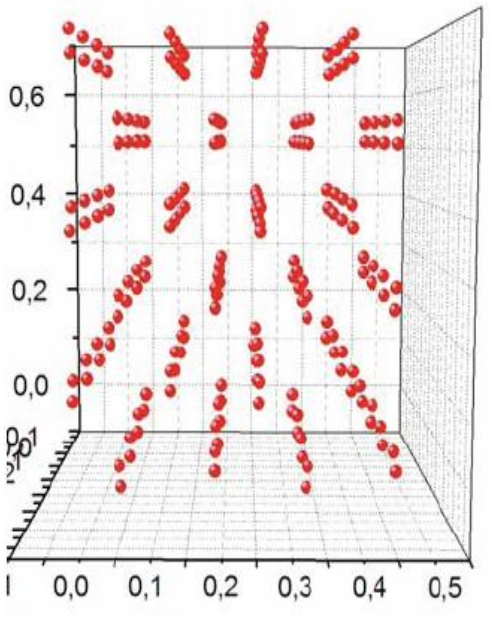
Crystal Structure

XCrysDen program

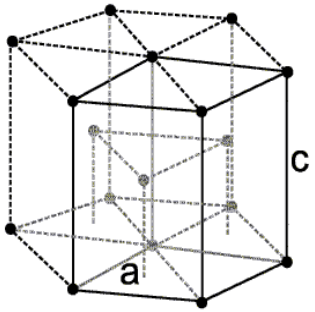




(b)

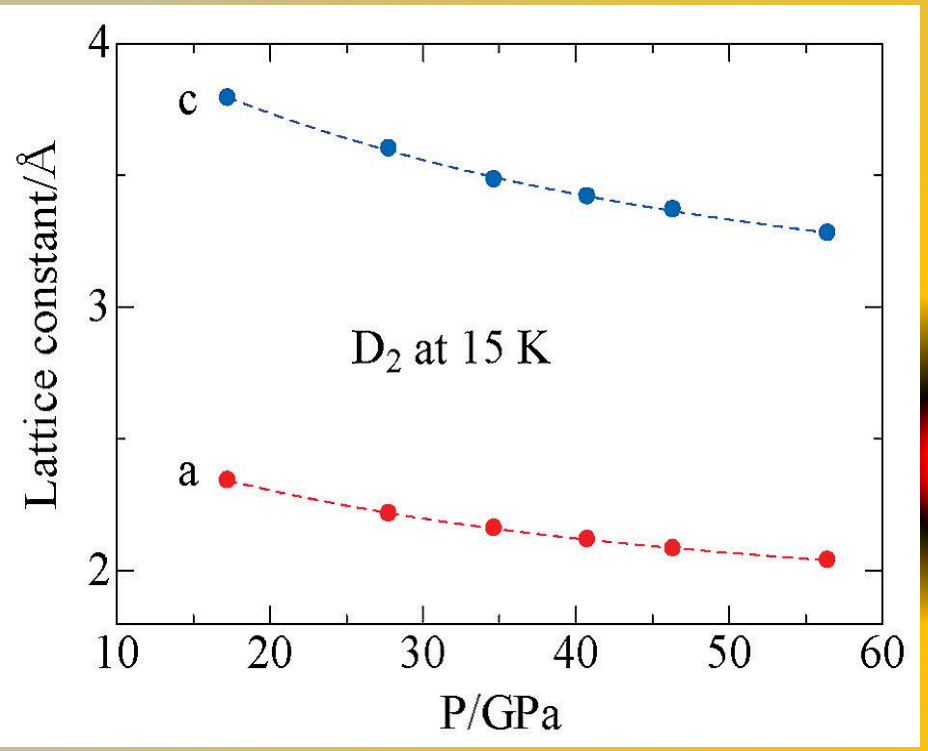


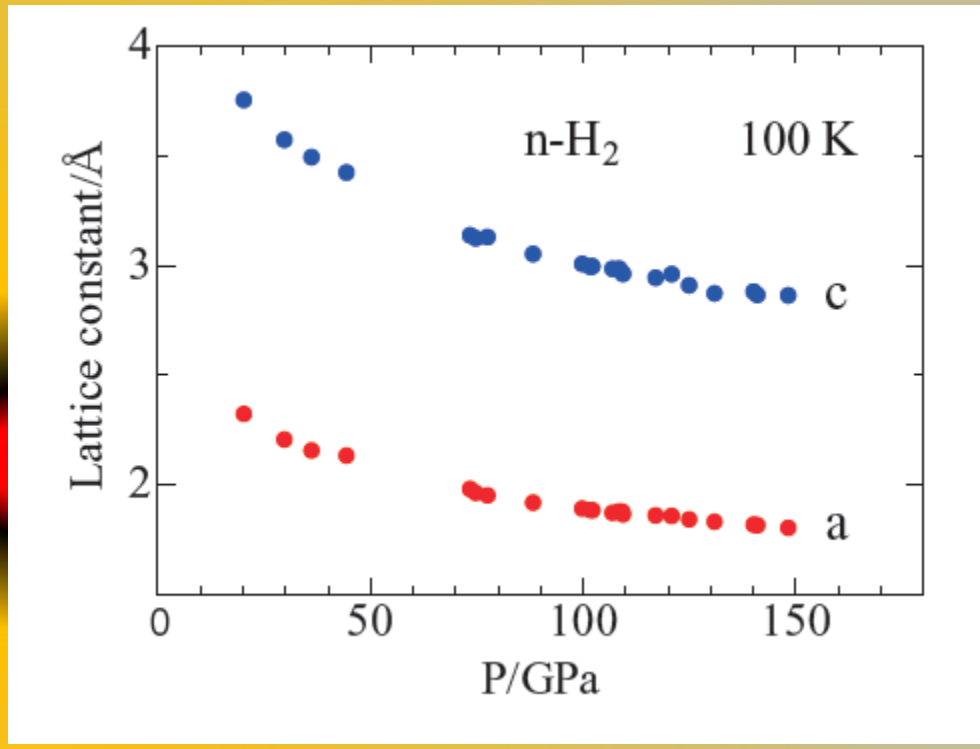
Crystal
HCP



(a) Various combinations that a hydrogen molecule is able to form with its isotopes, hydrogen (H), deuterium (D) and Tritium (T). (b) The distribution of molecules, each pair can be a different mix, is therefore an important factor to consider, in addition to the isotope mixture in the sample.

Lattice constant





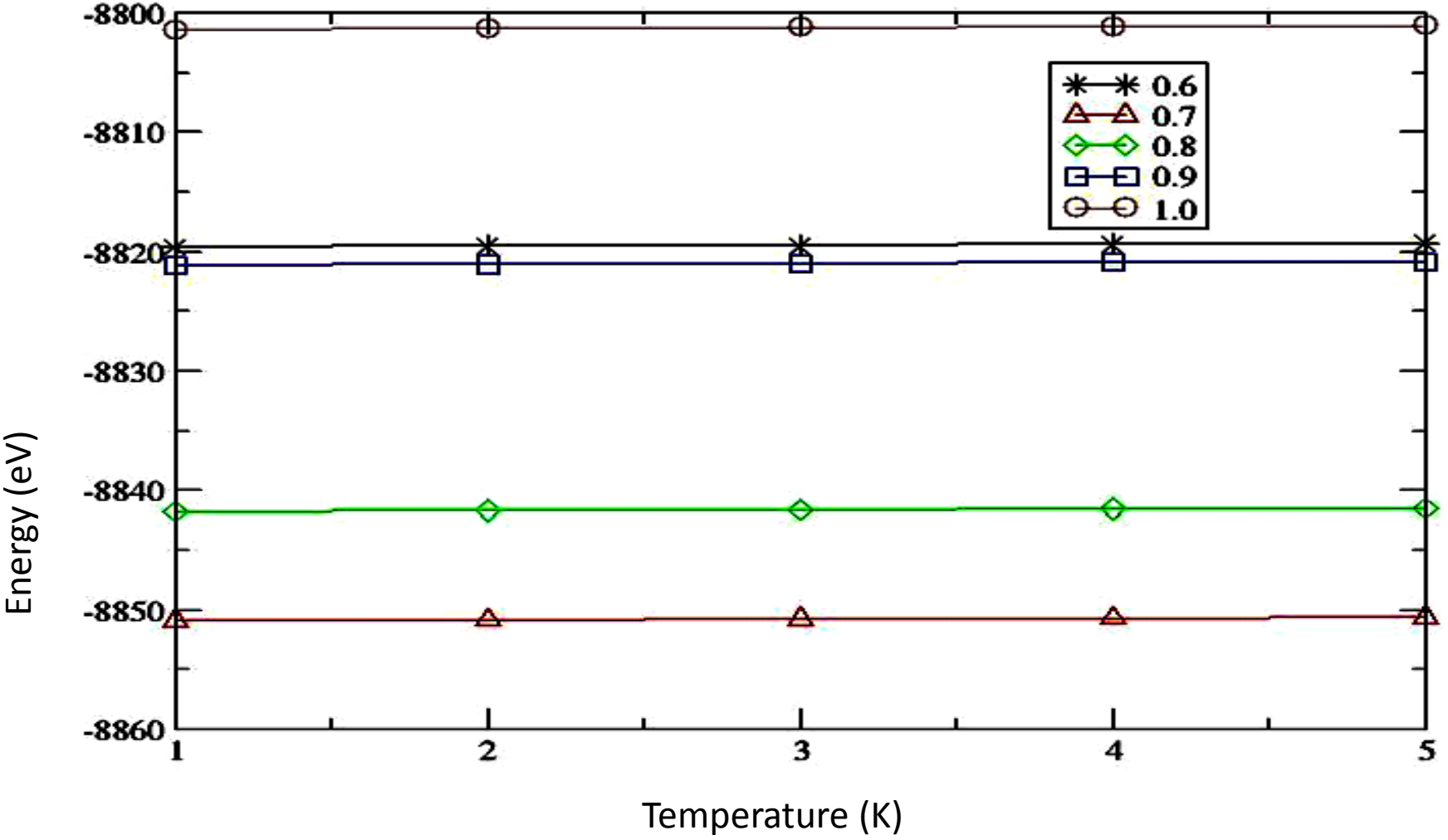
Kawamura 2008

lattice parameter varies with the molar volume (Souers 1984),

$a=1.329 \times 10^{-8} Vs^{1/3}$

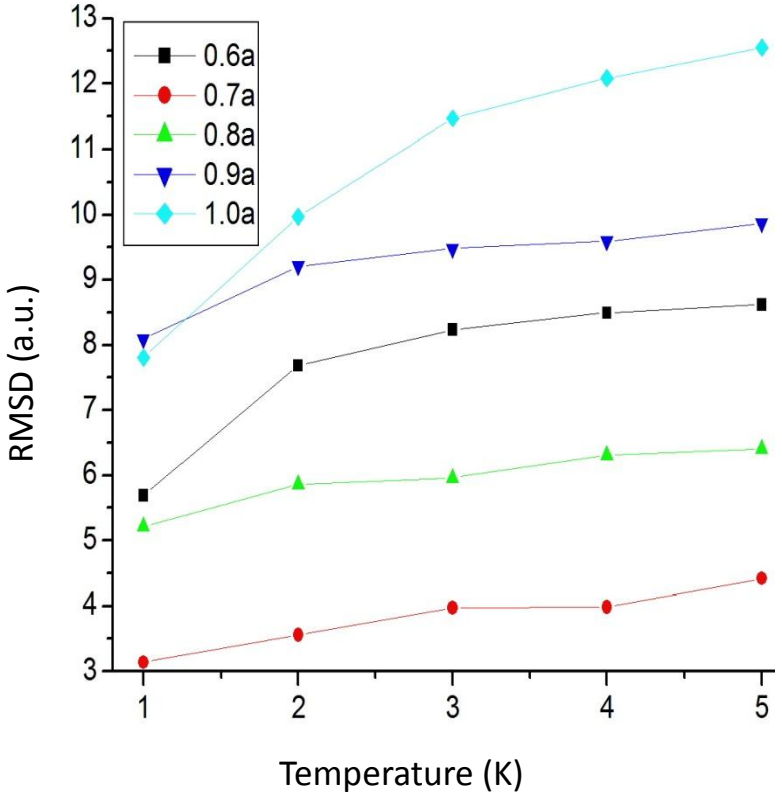
Inicials Conditions

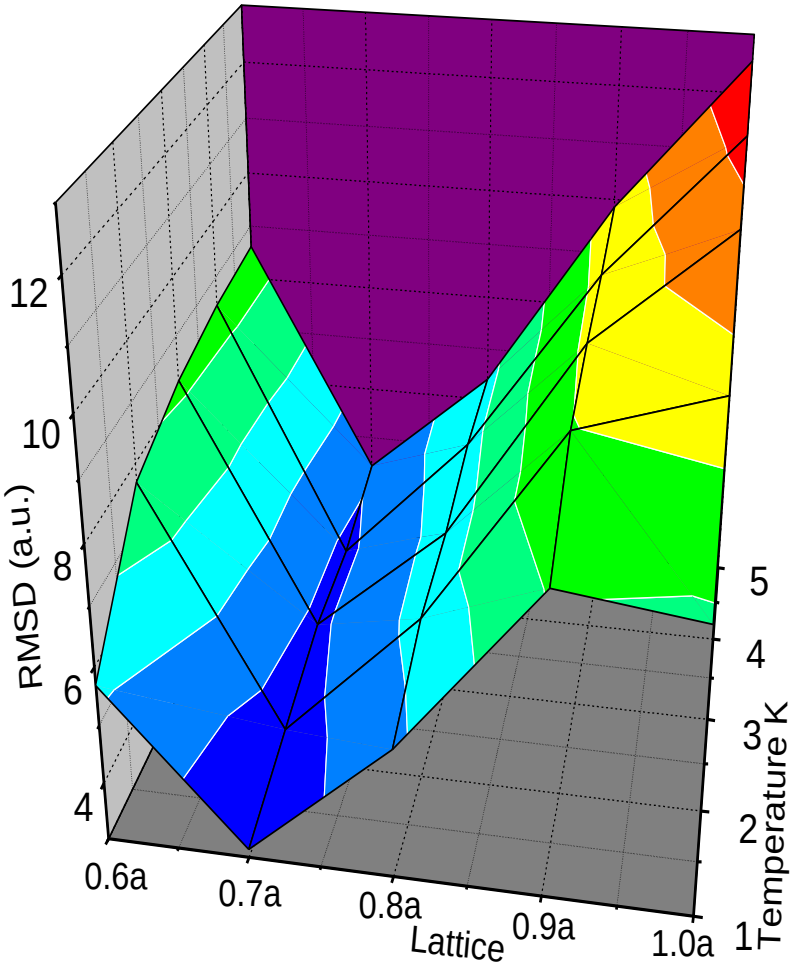
Energy



a= 3.783 Å (Souers 1986, Galtsov 2003). In this imagen *0.9= 0.9 x a,* equal *0.8 - 0.7…*
Nose-Hoover Thermostat with zero pressure for five temperatures

RMSD: Root Mean Square Deviation

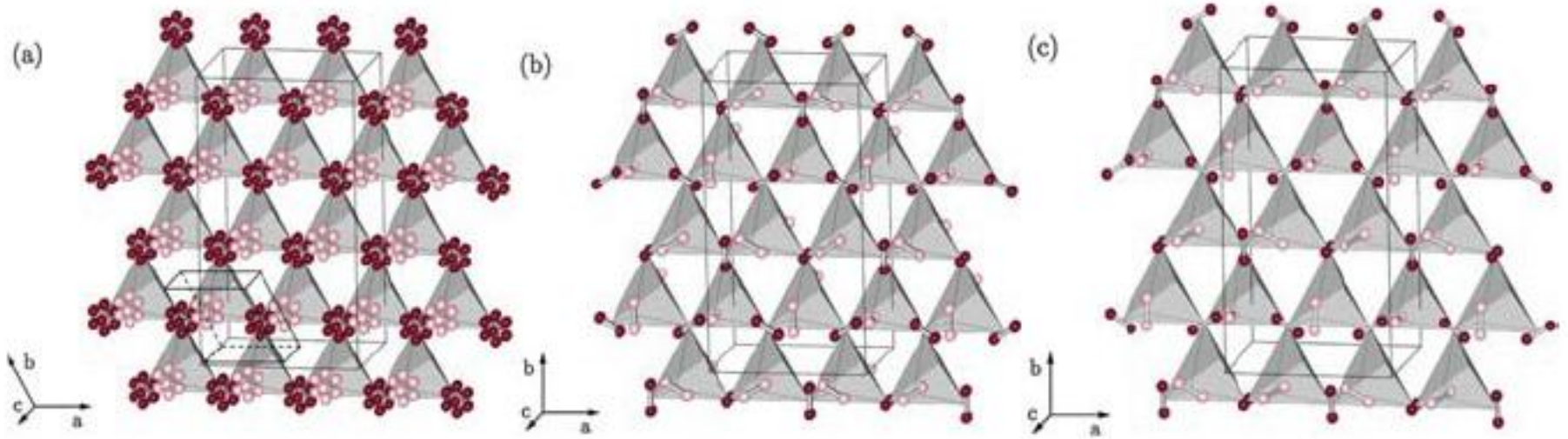




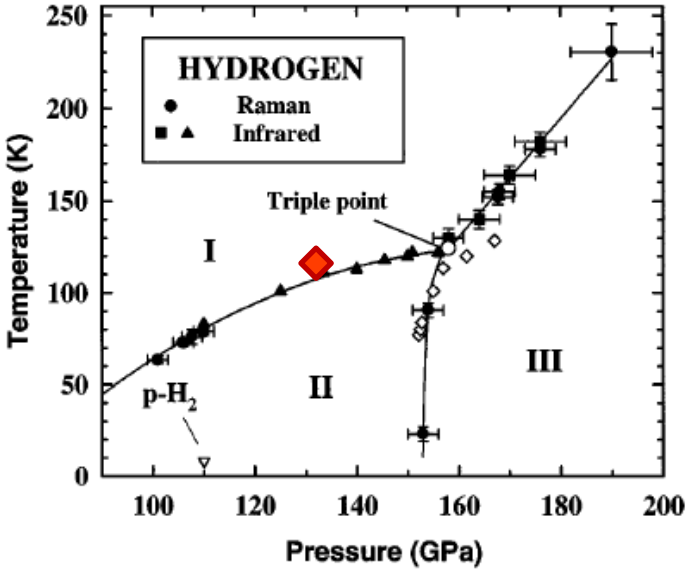
RMSD, difference between initial and final structural configuration

Phase Transition

Toledano 2009

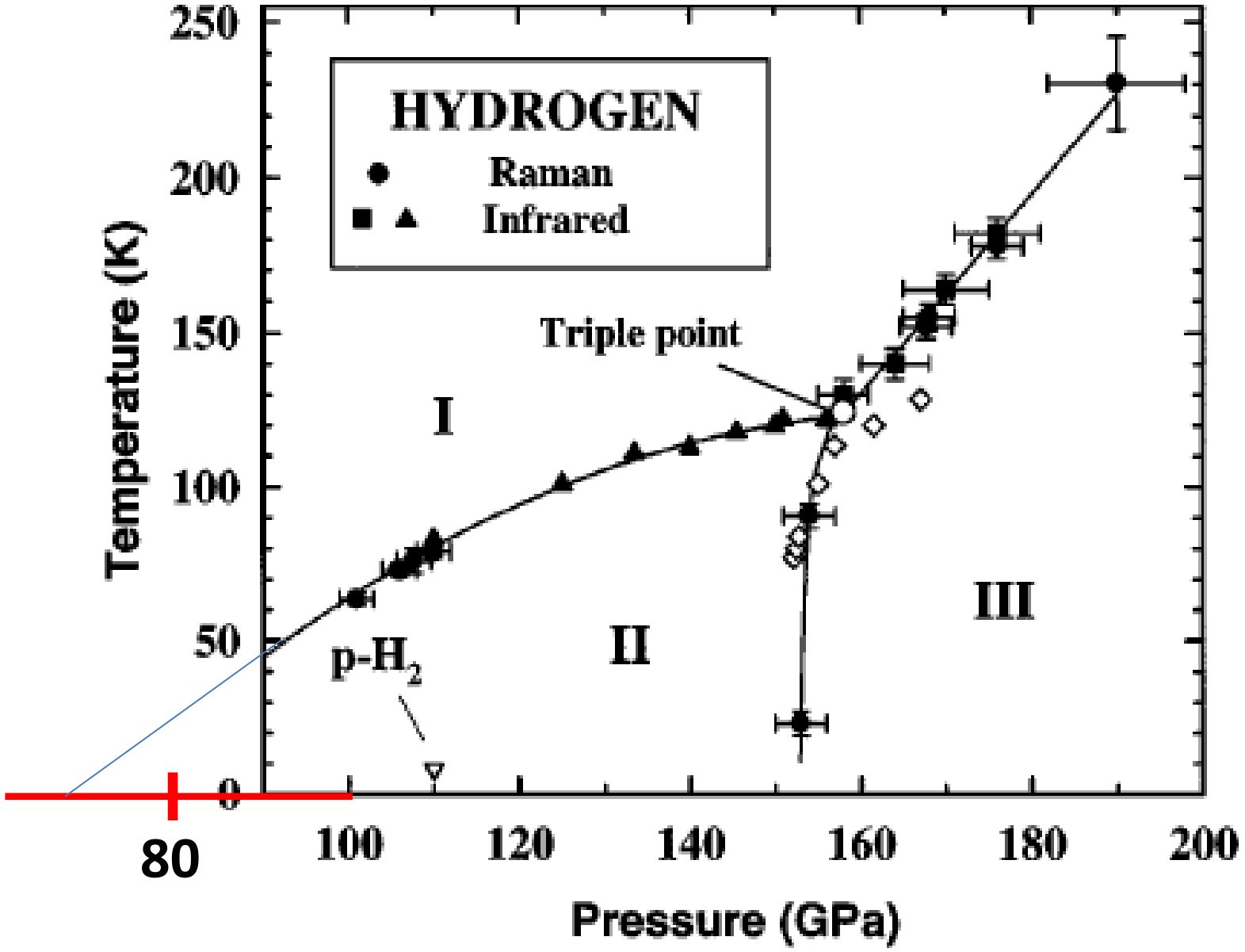


PHASE I PHASE II PHASE III

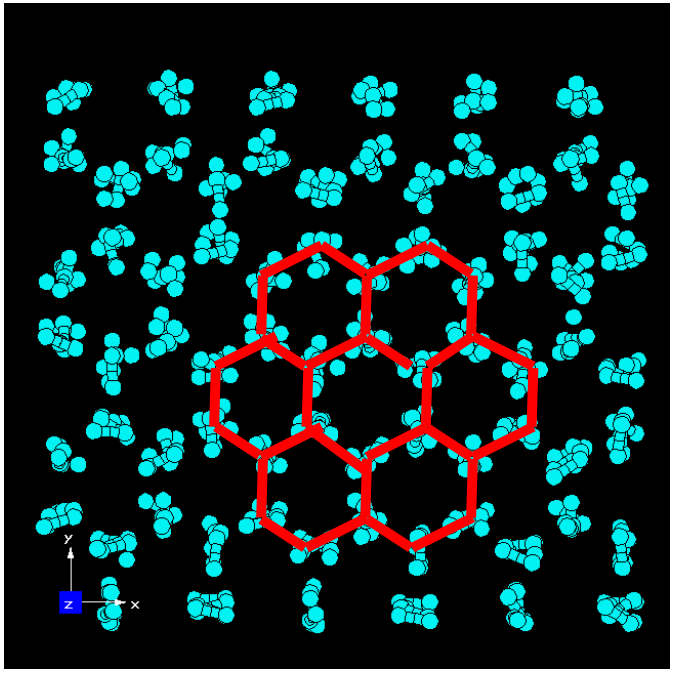


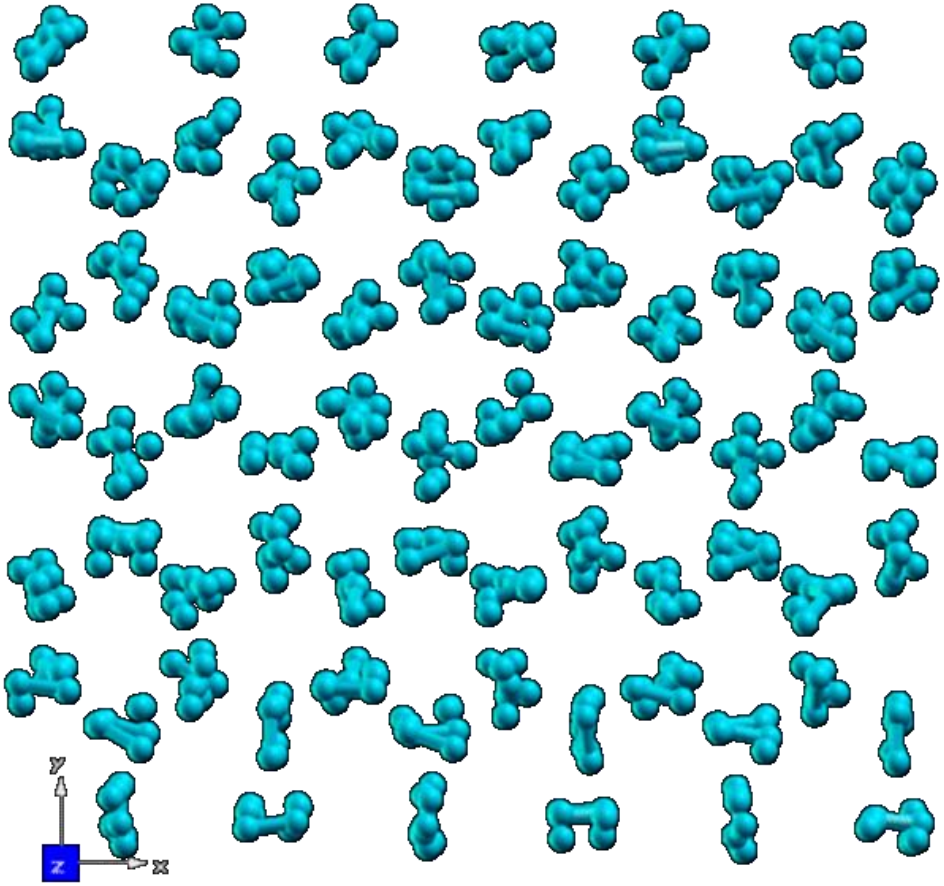
We observe the models described by Toledano et al for the three phases of solid molecular hydrogen. The Phase I to II transition near 110 GPa, while we observe it much lower below 80 GPa, this is because to simulate para - hydrogen ($p\text{-}H_2$).

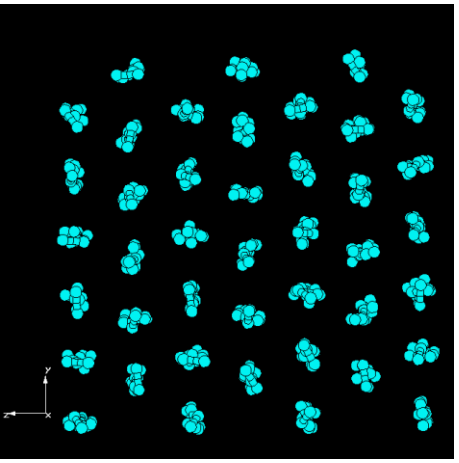
Mazin 1997

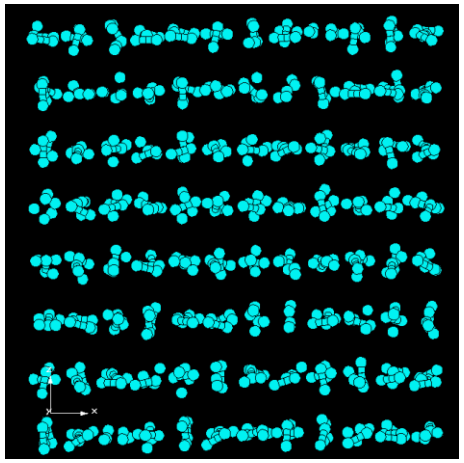

HYDROGEN
Raman
Infrared
Triple point
I
II
III
p-H2
Temperature (K)
Pressure (GPa)
250
200
150
100
50
0
100
120
140
160
180
200
80

Hydrogen 15K 1GPa 1ps

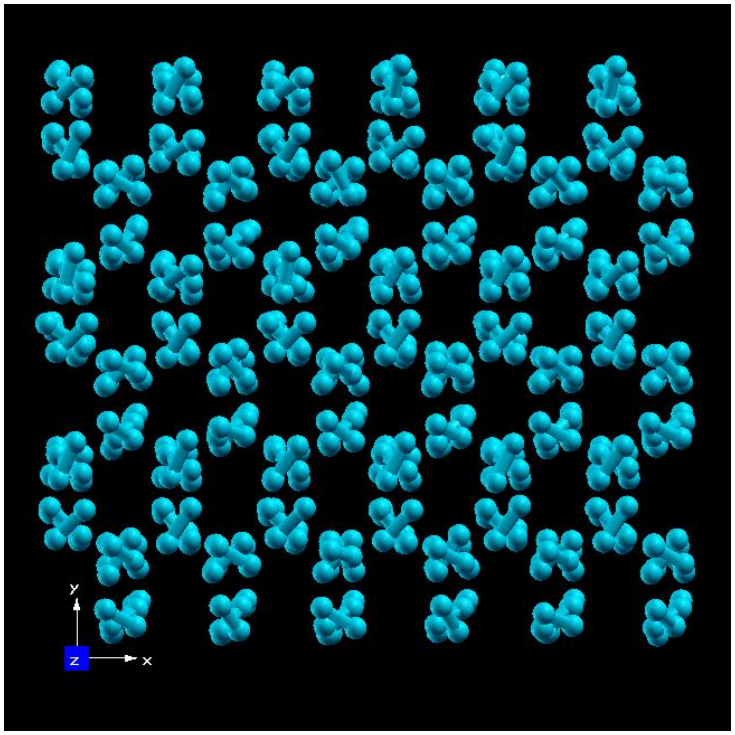


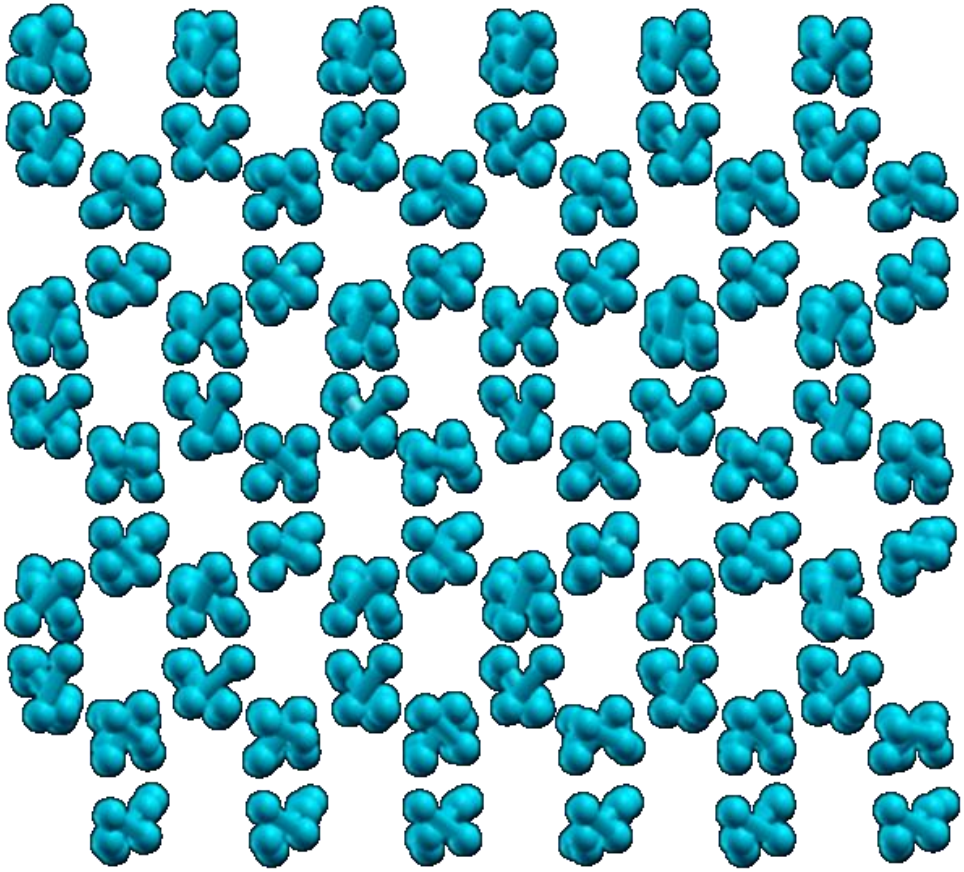


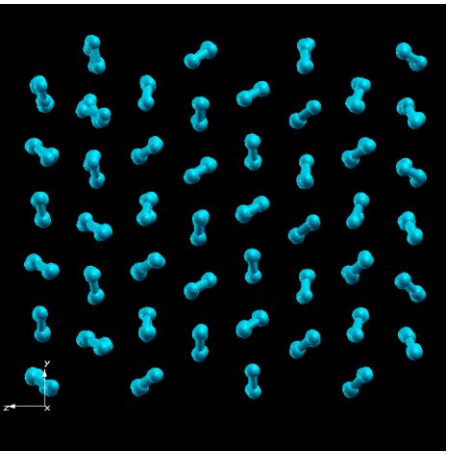


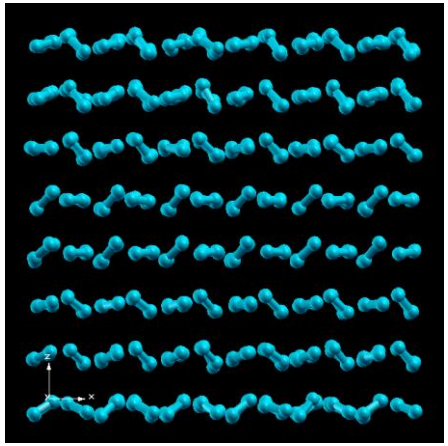


Hydrogen 15K 45 GPa 1 ps

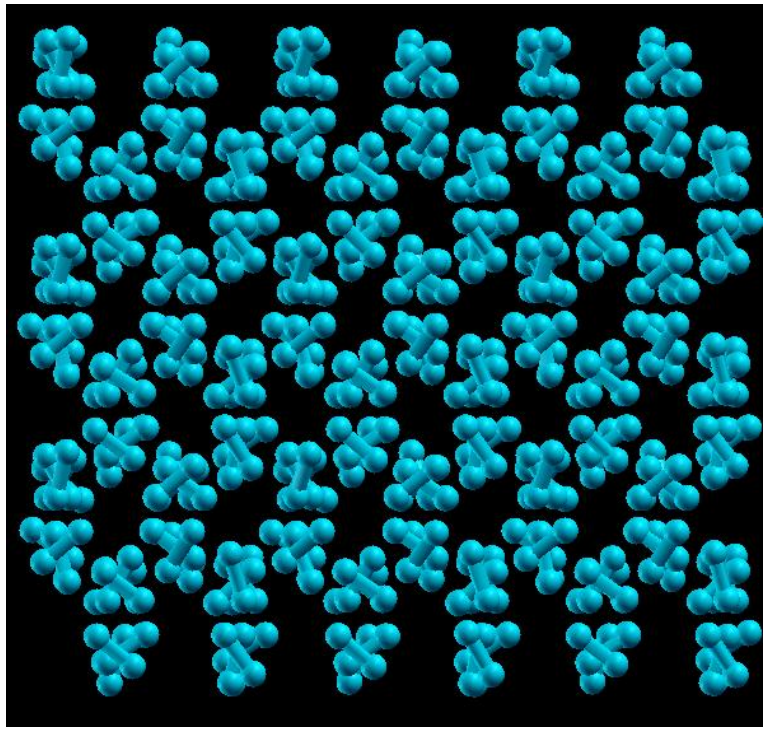


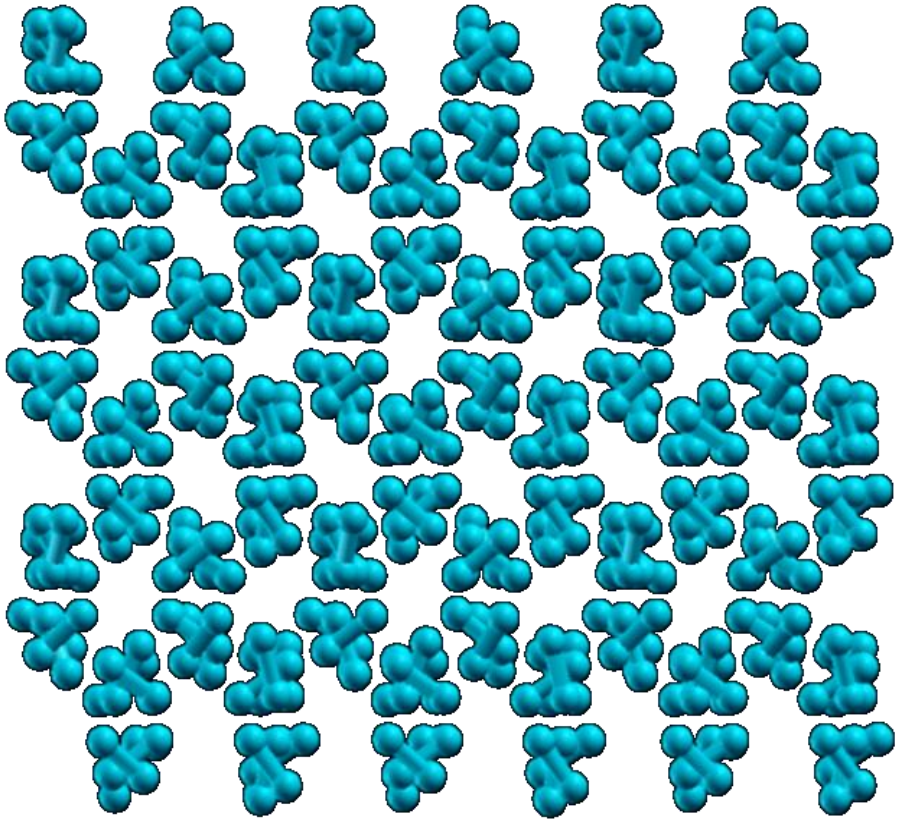


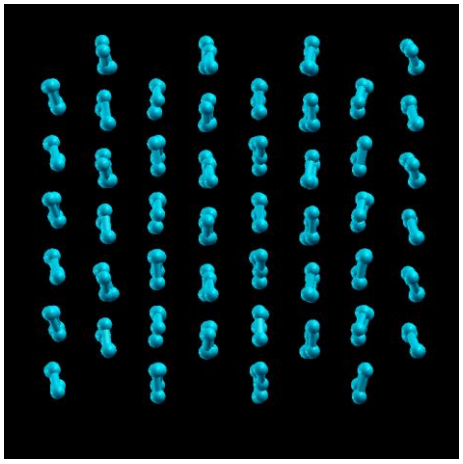


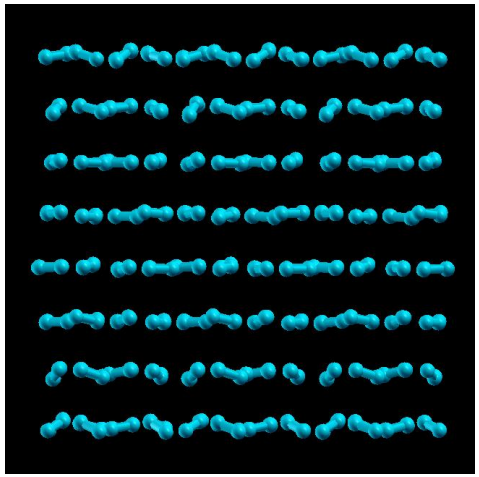


Hydrogen 15K 80 GPa 1 ps

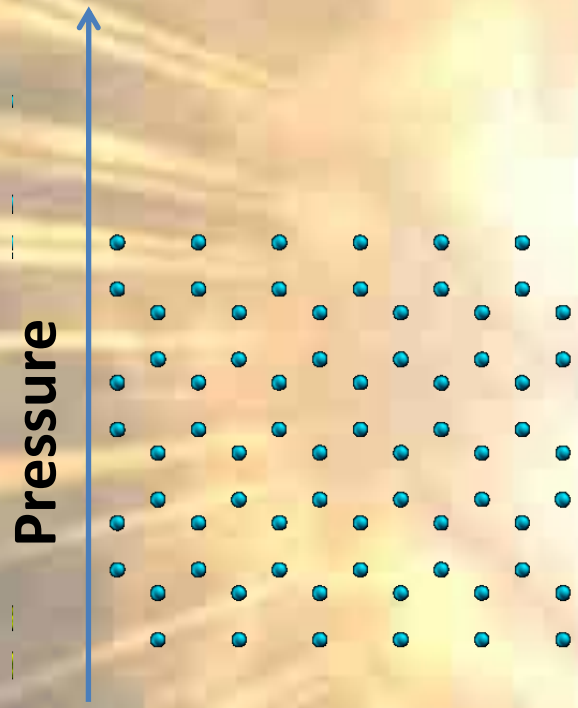


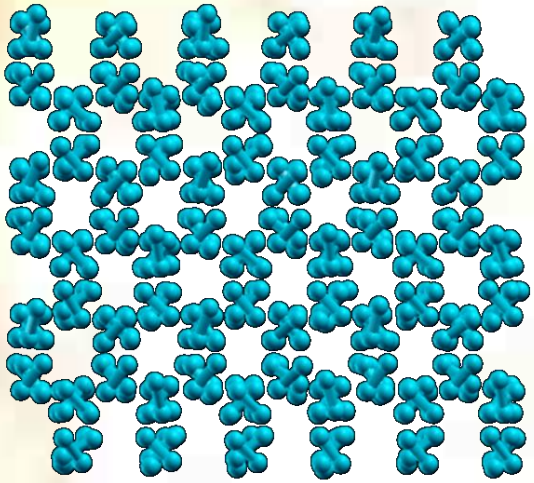






Ramps





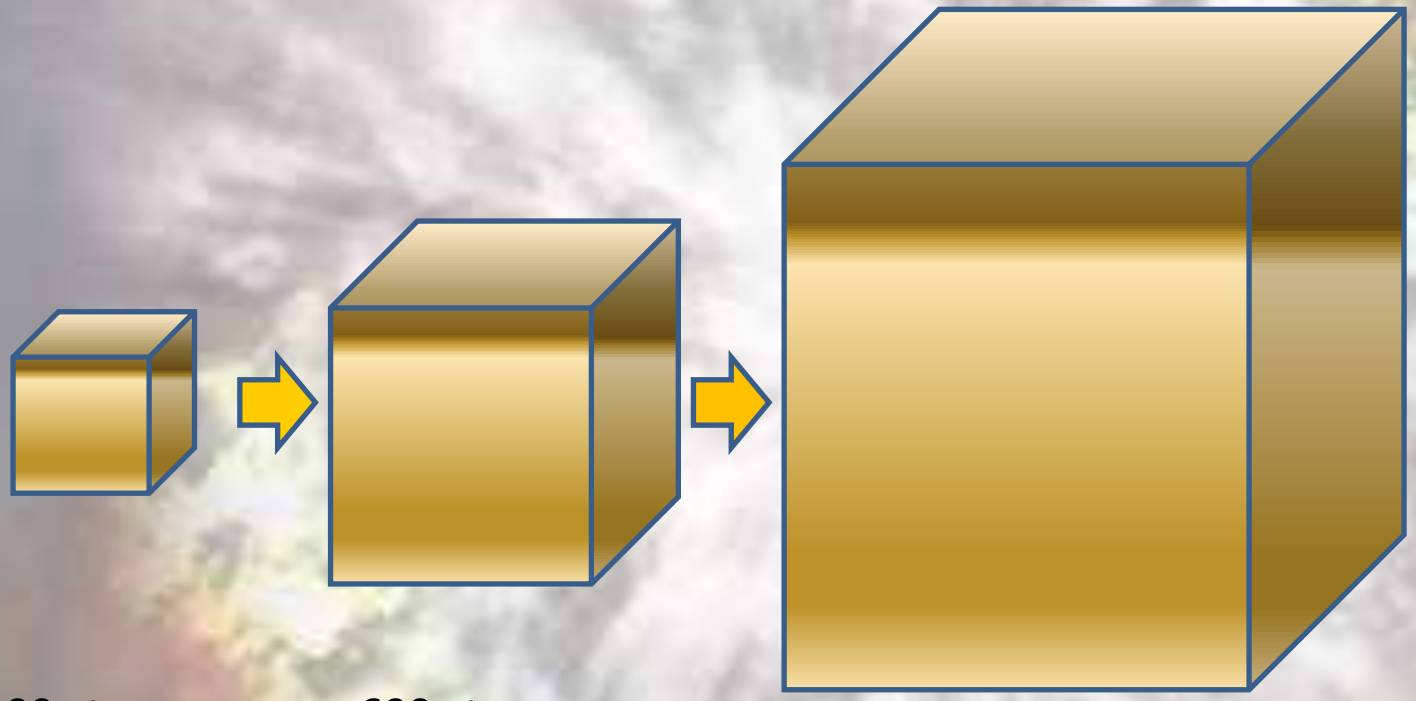
to reach a
certain pressure is
increased in steps

Nose – Hoover *Thermostat*
Parrinello – Rahman *Barostat*

P=0

Nose – Hoover
Thermalization

Size Scaling of Simulation



DM with potentials generated by *ab initio* methodology

~200 atoms

Preliminary studies

~600 atoms

Present Results

To H_2 , D_2 , T_2

Next:

HD, DT, HT and HDT

1000 – 2000 atoms

Future studies

parameters for engineering

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In this moment

	1GPa	2GPa	3GPa	4GPa	5GPa	7GPa	10GPa	15GPa	20GPa
H 15K									
D 15K									
T 15K									

25GPa	30GPa	35GPa	40GPa	45GPa	50GPa	60GPa	70GPa	80GPa	90GPa

100GPa	110GPa	120GPa	130GPa	150GPa	170GPa	200GPa	250GPa	300GPa	500GPa

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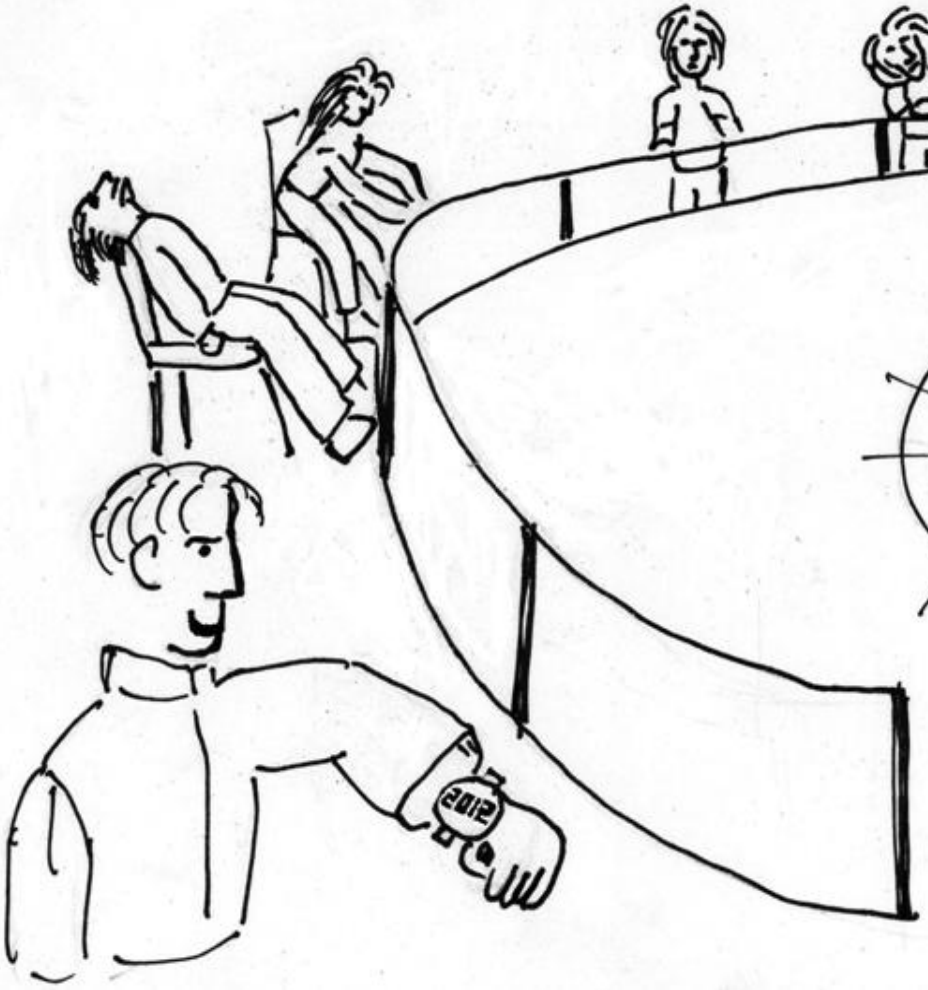
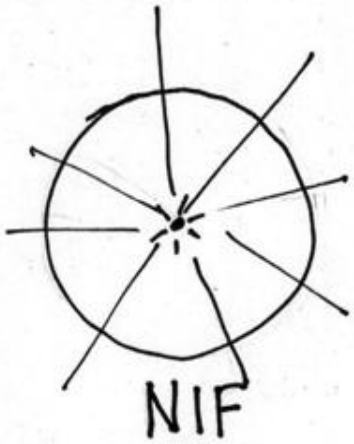
Conclusions

- We have a method of multiscale simulation by which describe the behavior of hydrogen and its isotopes, varying the pressure and temperature, observing the structural changes.
- We observed phase transitions of hydrogen from Phase I to Phase II, close to 80 GPa, which differ as calculated by Toledano et al, but is consistent with the experiments of Mazin et al. Being satisfied with the behavior of para-hydrogen.





THANK YOU

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REFERENCES

I V Aleksandrova et al.Journal of Physics D: Applied Physics, 37, 1163–1178 **(2004).**
D. R. Harding, et al. LLE Review, Quarterly Rept., 99, 160 **(2004).**
B. J. Kozioziemski, et al. Physical Review B, 82, 012104 **(2010)**
I.V Alekxandrova et al.Journal of Russian Laser Research, Volume 28, Number 3 **(2007).**
H. Kawamura et al. The Review of High Pressure Science and Technology, Vol. 18, No. 1 **(2008)**
I.F. Silvera et al. Journal of Physics: Conference Series 215 012194 **(2010).**
P. Toledano et al. Physical Review Letters 103, 105301 **(2009)**
P.C. Souers. Hydrogen Properties for Fusion Energy. University of California.**(1986).**
N.N. Galtsov et al. Fizika Nizkikh Temperatur. v. 29, Nos.9/10, p. 1036–1040 **(2003).**
Mc Mahon et al. Physical Review Letters 106, 165302 **(2011).**
Mazin et al. Physical Review Letters. Volume 78, Number 6 **(1997).**
Caillebet et al. Physical Review B 83, 094101 **(2011).**

Current Results and Perspectives

Simulation of the parameters of Hydrogen, Deuterium and Tritium.

Increased the number of atoms in the sample of the grain size, 1000 – 2000 atoms.

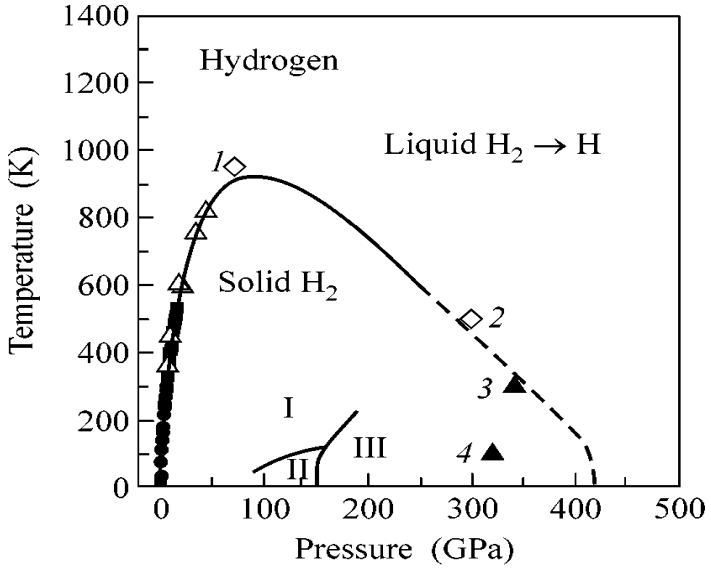
We search the properties for different ratios of HD, HDT, DT

We estimate the parameters needed to simulate the potential to build a larger scale structures Molecular Dynamics (LAMPPS or our original code), rising to the 40,000 molecules, for this we have the help of CESVIMA the UPM, as TOP500 *in number* 136, named *Magerit* with 4000 processors.

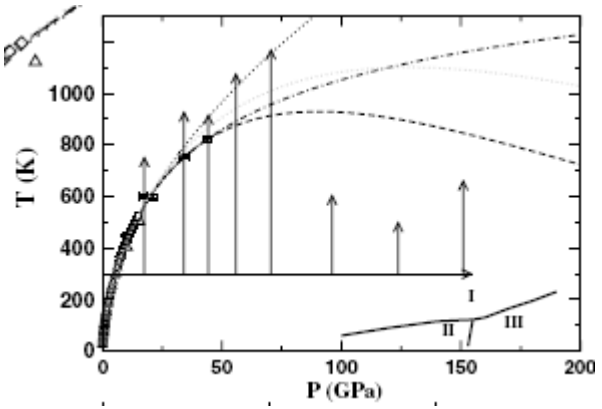
Knowing the crystal structures of the hydrogen isotopes at high pressures above 200 GPa. And for low pressures.

Build a more accurate equation of state from the multiscale approach with *ab initio* methods (Caillabet 2011)

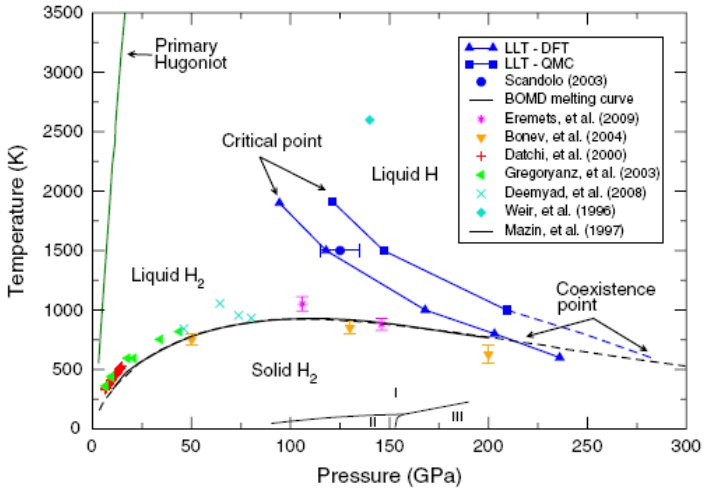
Phase Diagram for Hydrogen
Phase I, II, III



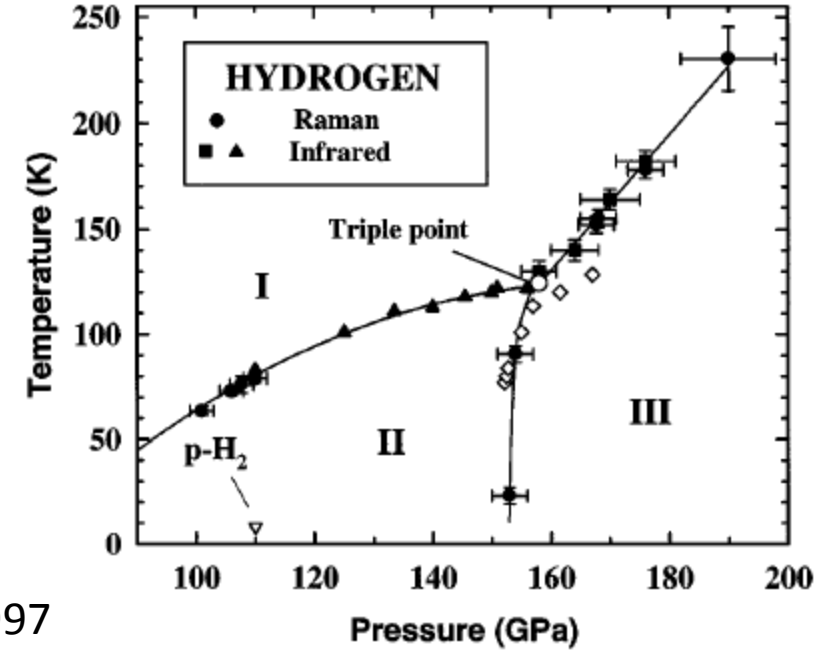
Kechin 2003



Gregoryanz 2003

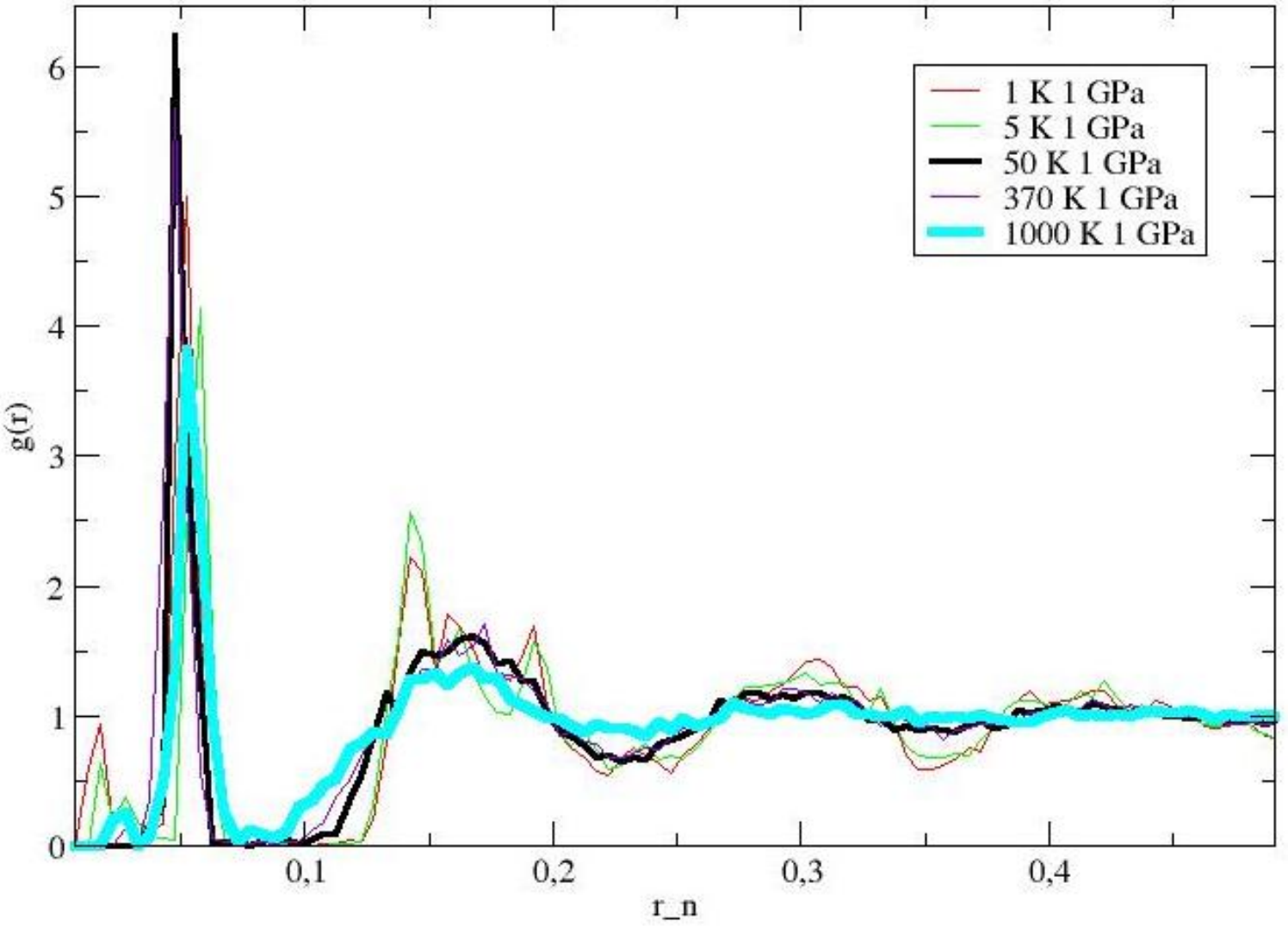


Morales 2010



Mazin 1997

G(r)


1 K 1 GPa
5 K 1 GPa
50 K 1 GPa
370 K 1 GPa
1000 K 1 GPa
g(r)
r_n
0
1
2
3
4
5
6
0,1
0,2
0,3
0,4

2011: theoritical structure to P> 500 GPa

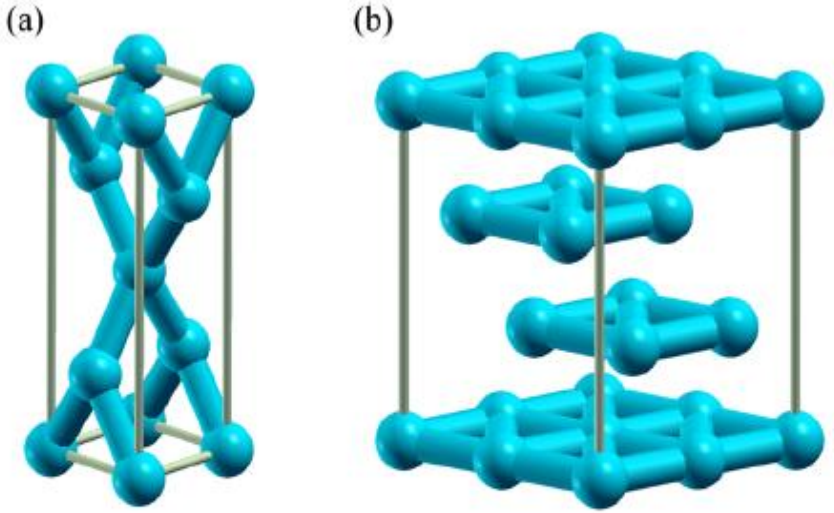


FIG. 2 (color online). Structures of the ground-state phases of atomic metallic hydrogen. (a) Unit cell of $I4_1/amd$ ($c/a > 1$). (b) $2 \times 2 \times 1$ supercell of R-$3m$. Fictitious bonds have been drawn for clarity.

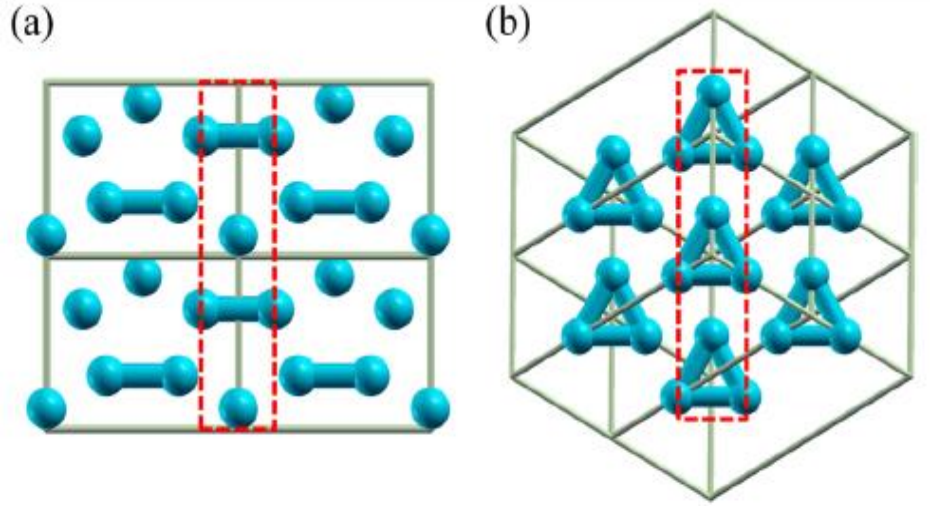
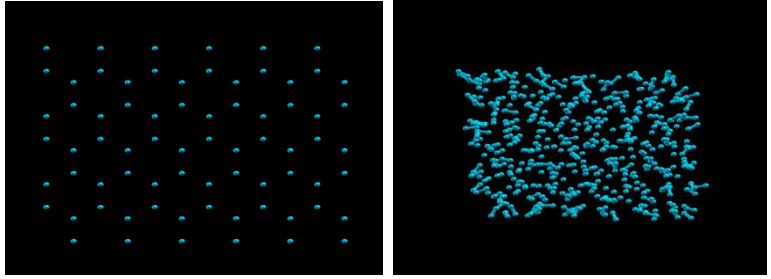
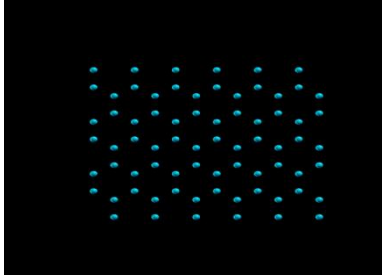
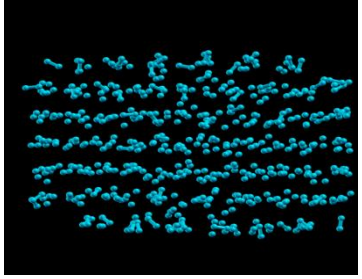


FIG. 3 (color online). Structures of (a) $Pmmn$ and (b) $R3m$. Note that the unit cells shown in (b) are actually $2 \times 1 \times 1$ supercells. The dotted lines border linear chains, which stick out of the plane relative to their neighbors.

McMahon 2011

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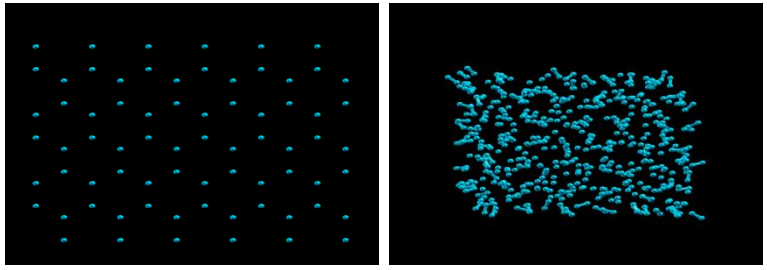
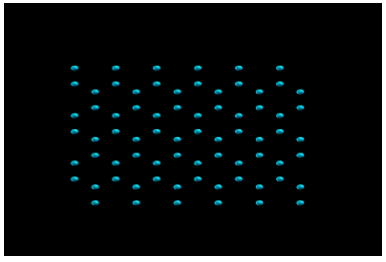
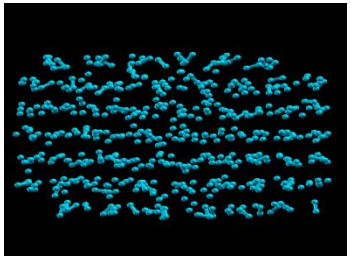

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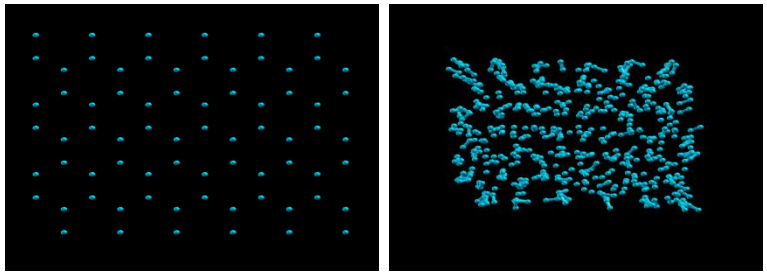
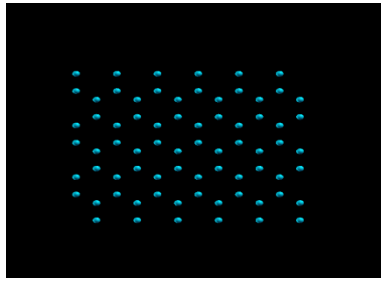
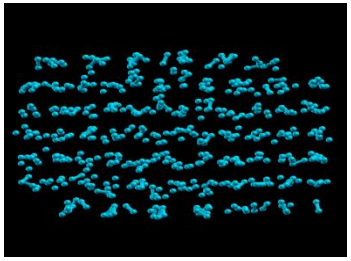

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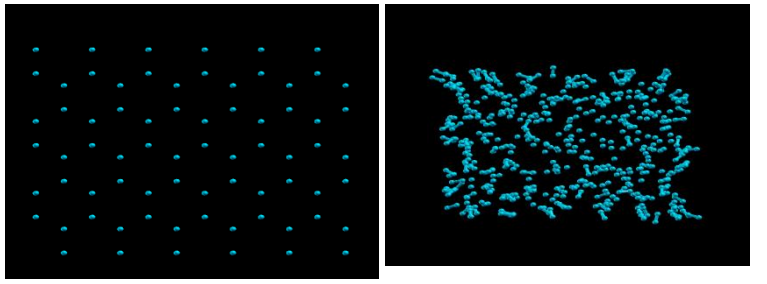
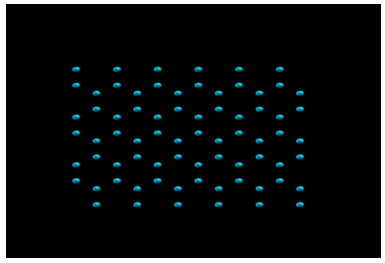
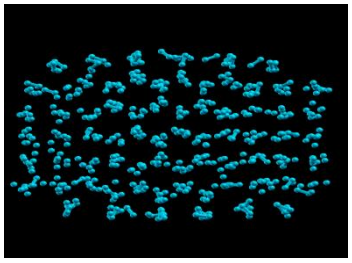

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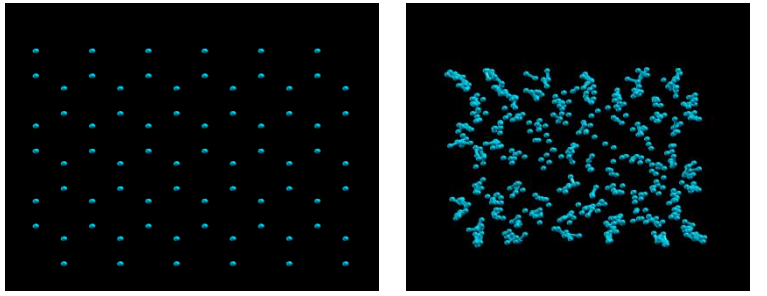
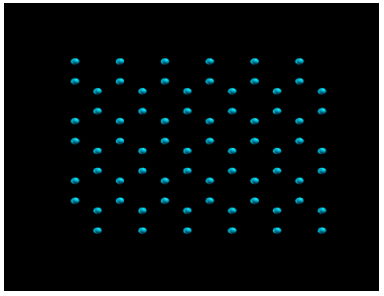
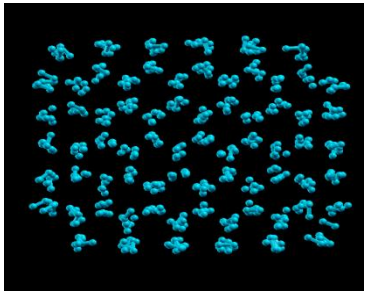

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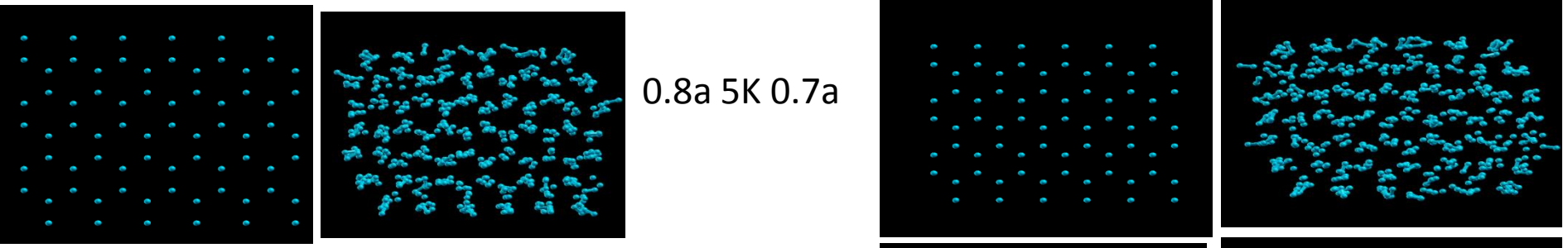
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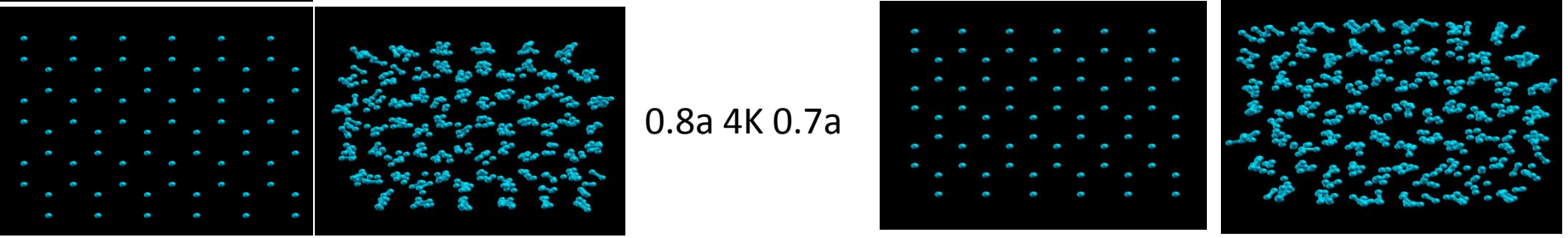
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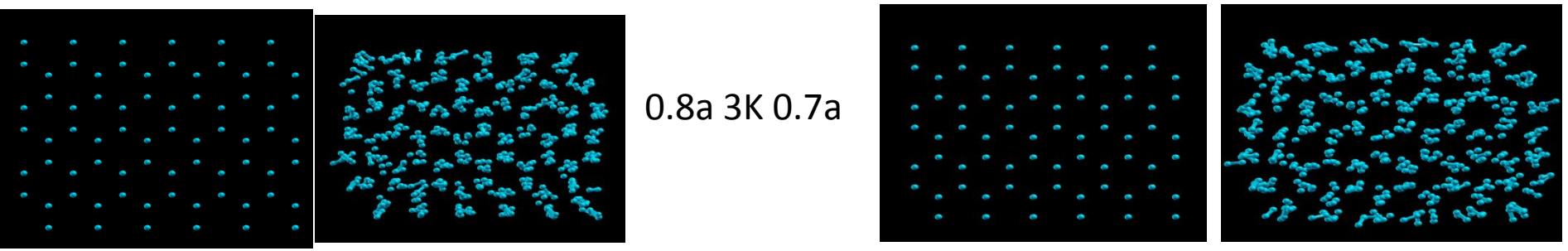
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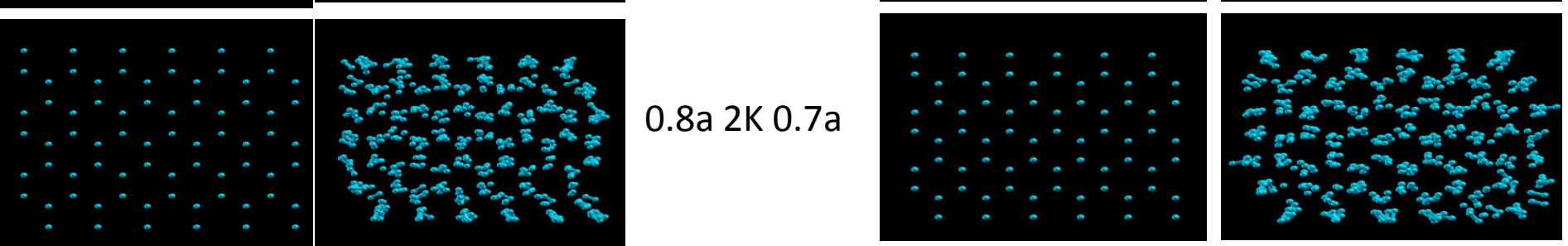
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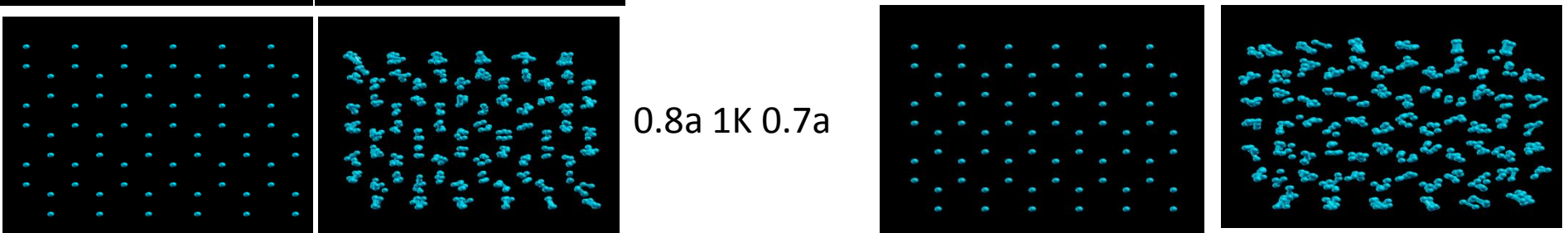
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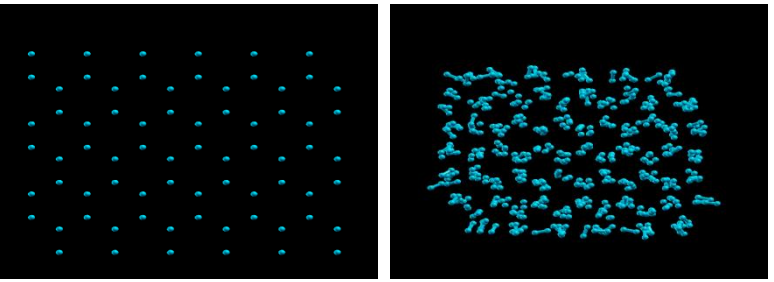

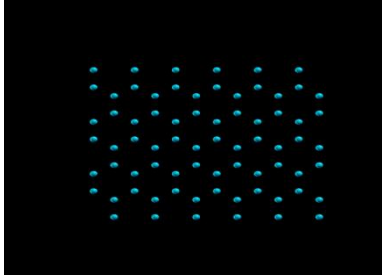
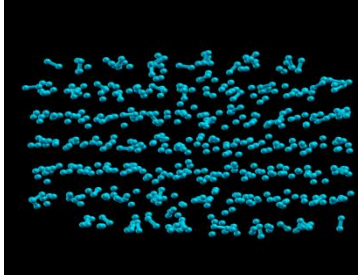

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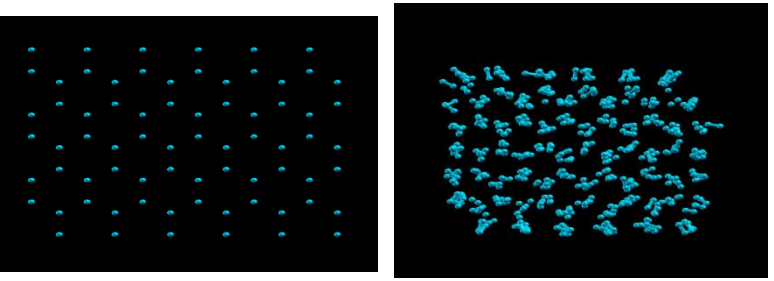

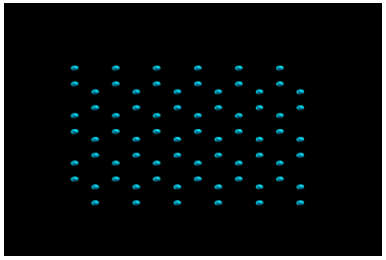
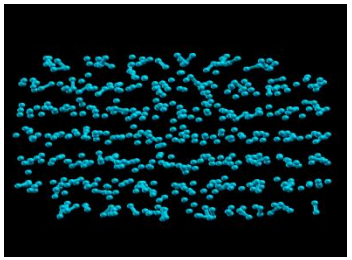

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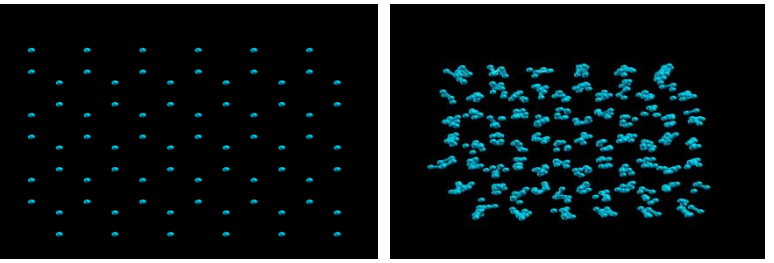

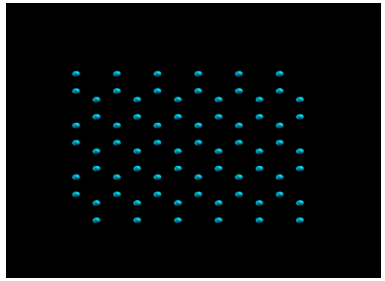
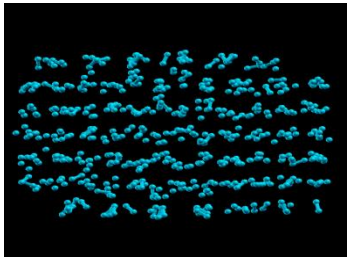

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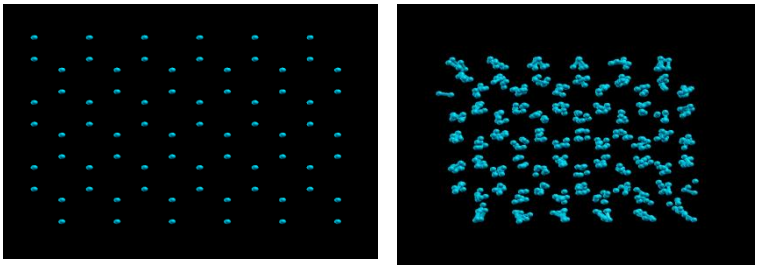

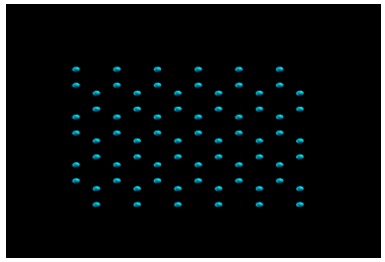
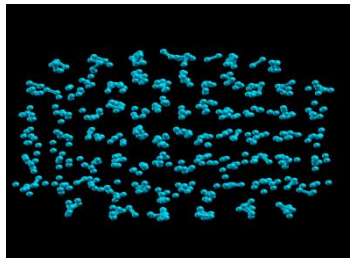

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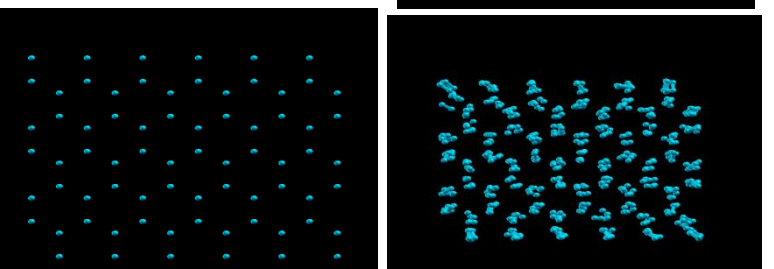
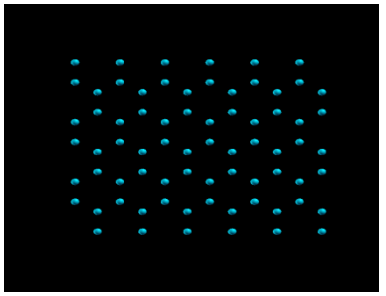
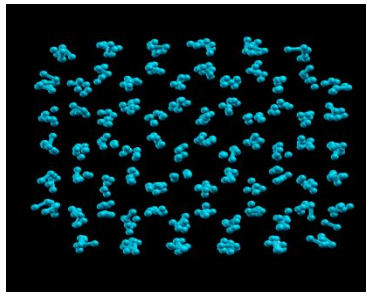
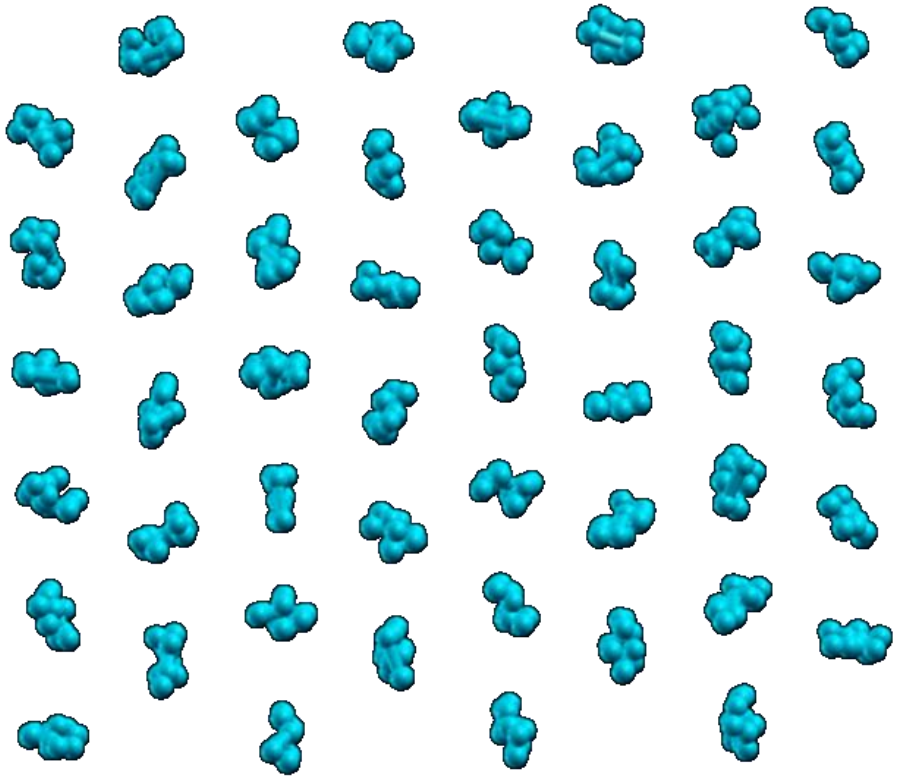
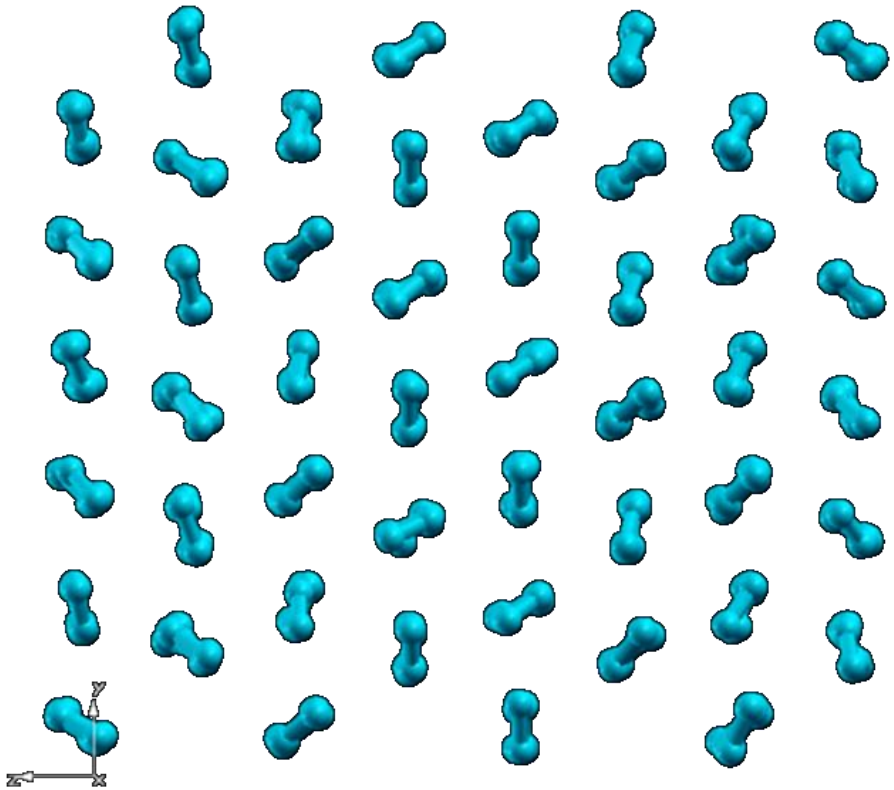


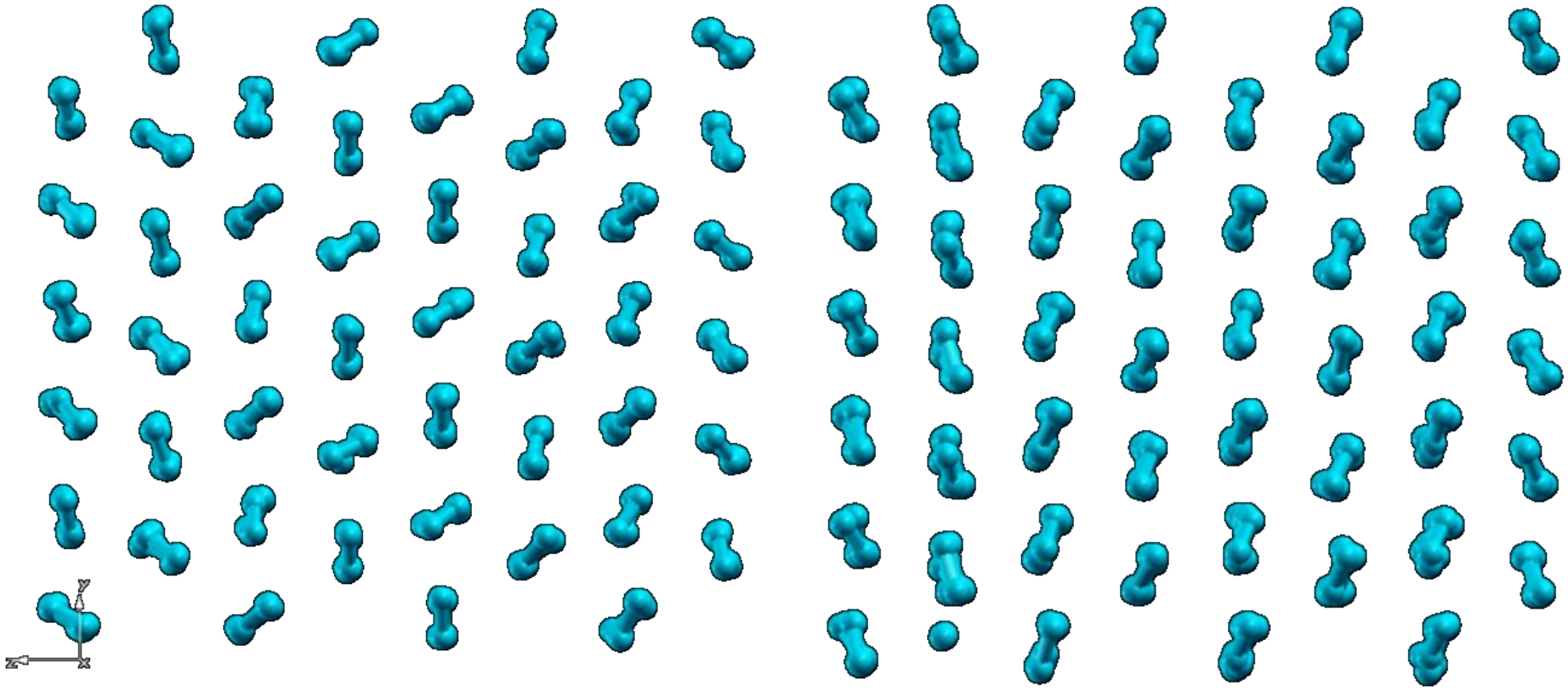
0.9a 1K 0.6a

1GPa and 45GPa to 15 K





45 GPa and 80 Gpa to 15 K



Para - hydrogen low 25 K

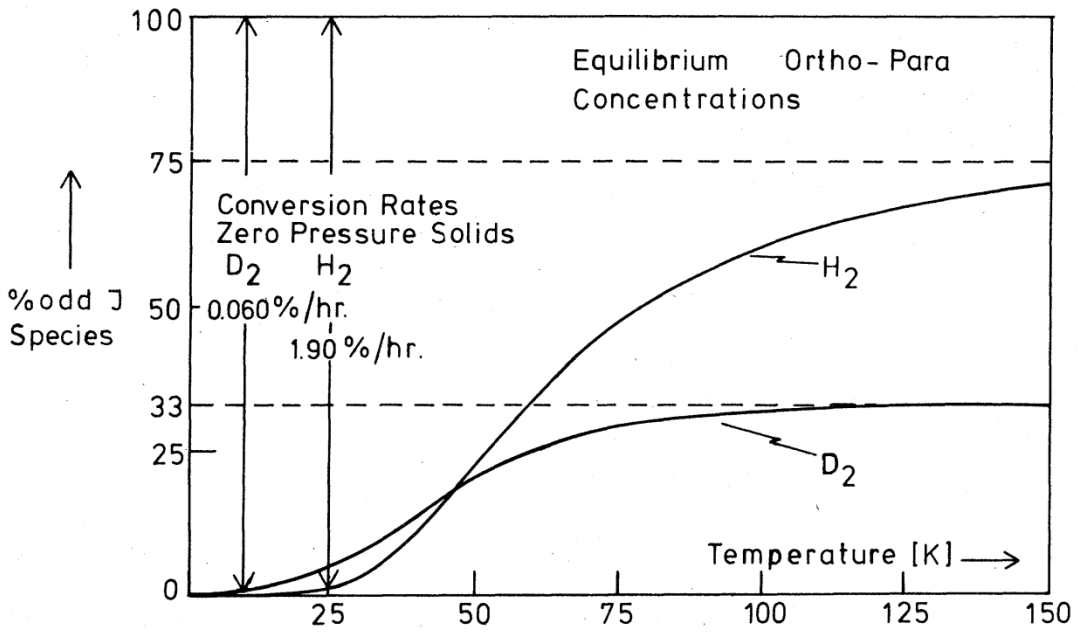


FIG. 15. Equilibrium ortho–para concentration of noninteracting hydrogen and deuterium as a function of temperature.

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Silvera 1980